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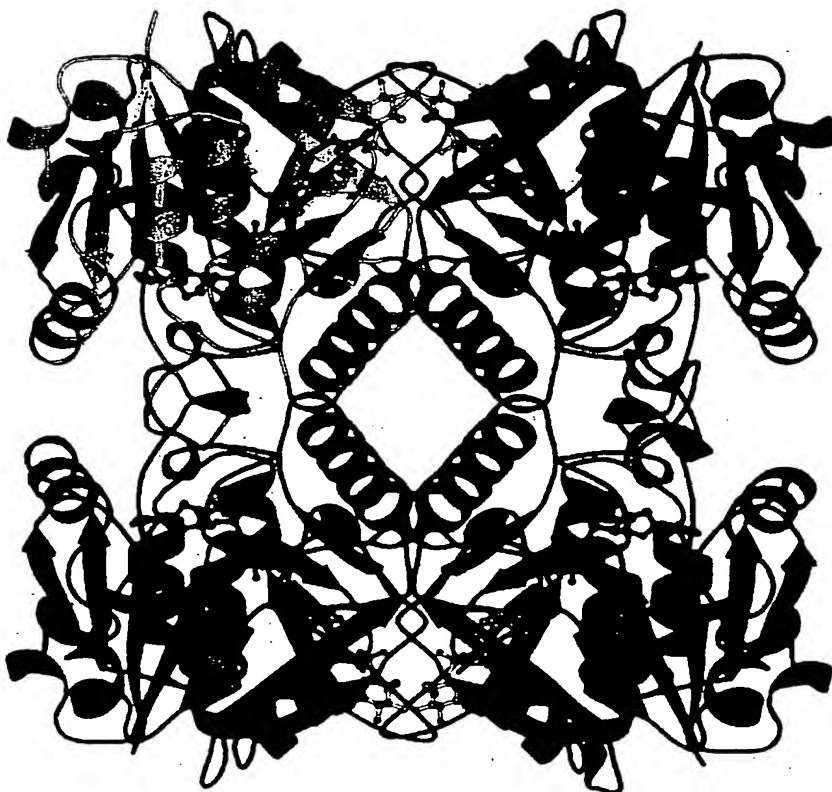
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(54) Title: **GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE AND METHOD FOR SELECTING INHIBITORS THEREOF**



(57) Abstract: There is provided a method of obtaining selecting agents which inhibit the enzyme glucose-1-phosphate thymidylyltransferase (RmlA) based upon analysis of a model of the active and regulatory site (s) of RmlA and interaction therewith by a potential inhibitory agent. The invention is based upon the provision of information on the structure of RmlA obtained through X-ray diffraction studies since a crystallised form of RmlA was obtained for the first time. The purified and crystallised form of RmlA, obtained from *Pseudomonas aeruginosa* is also described.

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1 Glucose-1-Phosphate Thymidyltransferase and Method
2 for selecting inhibitors thereof

3
4 The present invention relates to the enzyme glucose-
5 1-phosphate thymidyltransferase (RmlA) and its use
6 in a method of selecting for agents which inhibit the
7 enzyme glucose-1-phosphate thymidyltransferase
8 (RmlA).

9
10 Bacterial cell-surface glycoconjugates are essential
11 for survival of pathogenic bacteria and for
12 interactions between bacteria and the host.
13 Consequently, there is reason to believe that
14 inhibitors directed against target reactions in
15 assembly of the cell-surfaces glycoconjugates may
16 provide viable alternate therapeutic approaches.
17 However, bacterial cell-surface glycoconjugates show
18 remarkable structural diversity due to variations of
19 the sugar components, linkages and substitutions. A
20 successful strategy requires identification of
21 enzymes and pathways unique to bacteria, yet present
22 within a wide spectrum of bacterial species. One

1 such target is the synthesis of the activated form of
2 L-rhamnose, dTDP-L-rhamnose.

3
4 L-rhamnose is a 6-deoxyhexose that is found in the
5 cell wall of many pathogenic microorganisms. In
6 Gram-negative bacteria it is one of the important
7 residues of the O-antigen of lipopolysaccharide, a
8 factor which is a key determinant for the virulence
9 of these species. In *Pseudomonas aeruginosa*, this
10 sugar is a constituent of the core oligosaccharide
11 and serves as the receptor for O-antigen polymer
12 (Rahim et al., 2000). Gram-positive bacteria such as
13 streptococci and mycobacteria, on the other hand,
14 utilise L-rhamnose in the arabinogalactan (AG) that
15 attaches the lipid mycolic acid layer to the
16 peptidoglycan layer (McNeil et al., 1990). It has
17 been demonstrated that this attachment is of vital
18 importance to mycobacteria: inhibitors of the
19 formation of the arabinan portion of AG, e.g.
20 ethambutol, can stop cell growth and are effective
21 drugs (see for example Deng et al., 1995). As L-
22 rhamnose is not found in mammals inhibition of its
23 biosynthetic pathway is a target of interest in the
24 development of novel antibiotics.

25
26 Four enzymes, glucose-1-phosphate
27 thymidyltransferase (RmlA), dTDP-D-glucose 4,6-
28 dehydratase (RmlB), dTDP-6-deoxy-D-xylo-4-hexulose
29 (RmlC) and dTDP-6-deoxy-L-lyxo 4-hexulose-4-reductase
30 (RmlD) are required for the synthesis of dTDP-L-
31 rhamnose from α -D-glucose-1-phosphate (G1P) and dTTP.

1 Significantly, these proteins are highly conserved
2 amongst microorganisms (see for example Ma *et al.*,
3 1997; Graninger *et al.*, 1999) and therefore
4 conclusions drawn from the structure of a protein
5 from one species will have strong implications for
6 the corresponding enzyme of another origin.

7
8 *Pseudomonas aeruginosa* is a Gram-negative bacterium
9 that colonises many children with cystic fibrosis
10 where it is a significant cause of morbidity and
11 mortality. In addition it is an opportunistic
12 pathogen that can cause a wide variety of infections,
13 particularly in victims of severe burns and in
14 patients who are for any reason immunosuppressed.
15 This makes *Pseudomonas aeruginosa* one of the most
16 prevalent pathogens in hospital-acquired infections.
17 Due to its high resistance to antibiotics it is a
18 particularly dangerous pathogen and any approach
19 towards its control is highly sought.

20
21 RmlA (glucose-1-phosphate thymidyltransferase, E.C.
22 2.2.7.24) catalyses the first of four steps in the
23 transformation of glucose-1-phosphate (G1P) to 2'-
24 deoxy-thymidyl-diphospho-L-rhamnose (dTDP-L-
25 rhamnose or dTDP-Rha) in a Mg^{2+} dependent manner (see
26 Figure 1). The reaction product, 2'-deoxy-
27 thymidyl-diphospho-D-glucose (dTDP-Glc), can also
28 be back-pyrophosphorylysed by RmlA, yielding 2'-
29 deoxy-thymidyl-triphosphate (dTTP) and G1P. It has
30 been demonstrated that the enzymatic activity of RmlA
31 is allosterically regulated by dTDP-Rha (Melo &

1 Glaser, 1965), making the protein a key player in the
2 biosynthesis of rhamnose. Hence, it presents itself
3 as an attractive target in the development of novel
4 antibiotics.

5
6 RmlA is of particular interest as it is not only
7 involved in the biosynthesis of L-rhamnose but also
8 in the pathways leading to other 6-deoxy sugars such
9 as L-talose or D-fucose as these share common
10 intermediates in the conversion of D-glucose to their
11 end-products (Nakano et al., 2000; Yoshida et al.,
12 1999). The enzyme is highly homologous to other
13 bacterial sugar nucleotide transferases (e.g.
14 glucose-1-phosphate uridylyltransferase). The sugar
15 nucleotide transferases catalyse the first step in
16 all sugar nucleotide chemistry and are of key
17 importance in biology and biotechnology. As RmlA
18 shows no sequence relationship to any protein
19 structure currently deposited in the PDB (Sussman et
20 al., 1998), it is expected to contain a novel fold.
21 It is not yet fully clear which reaction mechanism
22 RmlA and related enzymes follow. They may either
23 obey Theorell-Chance (Theorell & Chance, 1951) or
24 ordered sequential bi-bi kinetics with the nucleotide
25 triphosphate binding to the protein first (Paule &
26 Preiss, 1971). An oxygen of GlP's phosphate group is
27 then believed to carry out a nucleophilic attack on
28 the NTP α -phosphate group directly as has been
29 demonstrated by the inversion of stereochemistry on
30 thiosubstituted NTPs (Sheu & Frey, 1978; Figure 1).

1 Purification and crystallisation of RmlA enzymes from
2 various micro-organisms has been generally possible
3 but the crystals obtained proved to be of
4 insufficient quality for structural studies, such as
5 X-ray diffraction studies. Surprisingly, it has now
6 been found that it is possible to obtain crystals of
7 RmlA from *Pseudomonas aeruginosa*, and that crystals
8 are of sufficient quality to perform structural
9 studies.

10

11 The present invention provides a purified and
12 crystallised form of RmlA from *Pseudomonas aeruginosa*
13 and its X-ray structure.

14

15 The present invention further provides a method of
16 selecting agents which inhibit the enzyme glucose-1-
17 phosphate thymidyltransferase (RmlA), said method
18 comprising the steps of:

19

20 a) providing a model of the active or regulatory
21 site(s) of RmlA;

22

23 b) reviewing the structure of a potential
24 inhibitory agent for at least one of these
25 sites; and

26

27 c) analysing the potential interaction of said
28 agent in said site(s).

29

30 Optionally, said model may be in the form of a
31 computer data or graphic file, and will usually be

1 based upon the X-ray crystal co-ordinates of RmlA.
2 Numerous computer programs, including graphic
3 programs, now exist to facilitate the handling of
4 said X-ray crystal co-ordinates and mention may be
5 made of FRODO (version 0), Insight and SYBIL, and the
6 like.

7
8 Conveniently, the potential inhibitory agent may
9 itself be reviewed in the form of a model, for
10 example a computer data file. Thus, the interaction
11 between the enzyme and potential inhibitory agent can
12 be analysed through interaction of the models, and
13 conveniently may be calculated by computer.

14
15 The structure of the agent to be tested for RmlA
16 inhibitory activity may conveniently likewise be
17 reviewed and analysed in the form of X-ray crystal
18 co-ordinates or approximations thereof. Optionally,
19 the potential intermolecular interaction between the
20 agent under test and the active site of RmlA will be
21 analysed with the aid of a computer.

22
23 In a further embodiment, the present invention
24 provides a method of selecting an anti-microbial
25 (such as anti-bacterial or anti-fungal) compound,
26 said method comprising following the steps a) to c)
27 outlined above, and including the step of selecting
28 an agent that binds to an active or regulatory site
29 of RmlA sufficiently tightly to impede the
30 biosynthesis of rhamnose and thus growth of the
31 micro-organism. It is preferred that the anti-

1 microbial agent is particularly effective against
2 *Pseudomonas aeruginosa*.

3
4 In a preferred embodiment, the agent will include one
5 or more regions able to interact with one or more of
6 the amino acids of the active or regulatory sites
7 (and in particular the amino acids specifically
8 mentioned in the description of the active and
9 regulatory sites given below and in Figures 7 and 8)
10 to impede the biosynthesis of rhamnose.

11
12 For example, the agent may desirably comprise a
13 negative charge and the interaction with the active
14 site of RmlA will desirably include an association
15 between the negative charge of the agent and at least
16 one of the amino acids Arg 15 and Lys 25.

17
18 The agent may also be provided with thymidyl-like
19 moiety able to interact (e.g. form hydrogen bonds)
20 with Gly 10, Gln 82 and/or Gly 87.

21
22 The agent may also be provided with a glucose-like
23 moiety able to interact (e.g. form hydrogen bonds)
24 with Asn 111, Gly 146, Glu 161, Val 172 and/or Tyr
25 176.

26
27 The present invention will now be further described
28 with reference to the examples and figures in which:

29
30 **Figure Legends**

31

1 **Figure 1:** Shows the first step of the conversion of
2 glucose-1-phosphate (G1P) into 2'-deoxy-thymidylyl-
3 diphospho-L-rhamnose or DTP-L-rhamnose. The reaction
4 catalysed by RmlA transforms G1P and dTTP to dTDP-D-
5 glucose.

6
7 **Figure 2:** Is a photograph of RmlA crystals obtained.
8 These crystals have been grown in the presence of
9 dTMP.

10
11 **Figure 3:** $\kappa=180^\circ$ section of the self-rotation search
12 in the TMP dataset. Done with REPLACE (Tong &
13 Rossmann, 1997). Search angle: polar XYK;
14 orthogonalisation AXABZ

15
16 **Figure 4:** Table 1: Data collection statistics for
17 non-Se-labelled RmlA crystals.

18
19 **Figure 5:** Table 2: Data collection statistics for
20 MAD experiment on BM14.

21
22 **Figure 6:** Overall structure of the RmlA tetramer with
23 the location of active (dark) and regulatory (light)
24 binding site indicated by bound ligand. The bound
25 molecule is dTDP-Glc in all cases.

26
27 **Figure 7:** Interactions of dTDP-Glc in the active
28 center of RmlA. The hydrogen bonding network is
29 indicated by dashed lines. Hydrophobic contacts are
30 shown as lunes. Water residues are presented as cyan
31 spheres.

1 **Figure 8:** Interactions of dTDP-Glc in the regulatory
2 binding site of RmlA.

3
4 **Examples**

5
6 **RmlA overexpression and purification**

7
8 The open reading frame of the gene encoding RmlA from
9 *Pseudomonas aeruginosa* was amplified using PCR with
10 primers that incorporated a 5' *Nco*I and a 3' *Bam*HI
11 site to facilitate cloning into a modified pET23a(+)
12 vector (Newton & Mangroo, 1999). The plasmid also
13 contained a sequence coding for a 6xHis-tag on the N-
14 terminus of RmlA to allow an easy purification on
15 metal chelating columns. Expression involves the
16 IPTG (isopropyl- β -D-thiogalactoside)-inducible T7
17 promotor and ribosome-binding sites conferred by the
18 vector. The sequence of the amplified and cloned
19 gene was confirmed to be identical to the chromosomal
20 copy excepting the N-terminal 6xHis-tag.

21
22 In order to overexpress RmlA *E. coli* BL21(λ DE3) cells
23 transformed with the plasmid were grown at 310 K in
24 Luria-Bertani medium containing 100 μ g ml⁻¹
25 ampicillin until the OD₆₀₀ reached 0.6 - 0.8.
26 Expression of the protein was then induced by
27 addition of 1 mM IPTG. After further 3 h of culture
28 cells were harvested by centrifugation (20 min, 6,000
29 g, 277 K).

30

1 The cell pellet was resuspended in a lysis buffer
2 containing 20 mM Tris-HCl pH 8.5, 100 mM NaCl, 2 mM
3 DTT, 5 mM PMSF and 100 $\mu\text{g ml}^{-1}$ hen egg white
4 lysozyme. After 30 min incubation at room
5 temperature, the viscosity of the mixture was
6 decreased by the addition of DNase I (20 $\mu\text{g ml}^{-1}$) and
7 by sonication (five cycles of 1 min interrupted by 1
8 min periods on ice). The suspension was centrifuged
9 at 20,000 g and 277 K for 20 min and the supernatant
10 then brought to 20 % ammonium sulfate saturation.
11 After incubation on ice for 1 h a second
12 centrifugation (20 min, 20,000 g, 277 K) was carried
13 out and the supernatant then dialysed against two
14 changes of 1 litre 20 mM Tris-HCl pH 7.0, 20 mM
15 imidazole and 500 mM NaCl. The filtered protein
16 solution was passed through a POROS-MC column which
17 had been pre-loaded with nickel sulphate. Proteins
18 were eluted with a 20 to 500 mM imidazole gradient. A
19 protein with a molecular weight corresponding to RmlA
20 (~ 34 kDa) was found in a peak eluting at approx. 200
21 mM imidazole. Fractions corresponding to this peak
22 were pooled, concentrated with a 10 kDa cut-off
23 Amicon membrane and dialysed against two changes of 1
24 litre of 20 mM Tris-HCl pH 8.5 at 277 K containing 10
25 mM EDTA in the first change to remove contaminating
26 nickel ions. For further purification the protein
27 was applied to a POROS-HQ anion exchange column on a
28 BioCAD 700E Workstation. Elution was achieved with a
29 50 to 1000 mM NaCl gradient. RmlA eluted at a salt
30 concentration of 200 mM. Pooled fractions were
31 brought to a protein concentration of approx. 4 mg

1 ml⁻¹ as determined by Bradford assay (Bradford, 1977)
2 using bovine serum albumin as standard and then
3 dialysed against two changes of 50 mM Tris-HCl pH 7.5
4 at 277 K. Prior to crystallisation experiments DTT
5 was added to 4 mM and the solution filtered through a
6 0.2 µm membrane. This procedure typically yielded 30
7 mg of pure protein per litre of bacterial culture.
8 Small aliquots of the purified protein could be
9 stored at 255 K without deterioration for several
10 months without addition of cryoprotecting agents.
11 Selenomethionine labelling of *Pseudomonas aeruginosa*
12 RmlA could not be achieved in *met*⁻ B834(λDE3) *E. coli*
13 cells. Under all conditions tested the protein
14 formed inclusion bodies. Selenomethionine enriched
15 protein was therefore produced by inhibition of the
16 methionine biosynthesis pathway in *E. coli* BL21(λDE3)
17 (Doublie, 1997). Briefly, cells were grown in M9
18 medium (64 g l⁻¹ Na₂HPO₄ · 7 H₂O, 15 g l⁻¹ KH₂PO₄, 2.5 g
19 l⁻¹ NaCl; 5 g l⁻¹ NH₄Cl, 1 mM MgSO₄, 0.4 % glucose, 0.1
20 mM CaCl₂) at 310 K until OD₆₀₀ reached 0.6. At this
21 stage the amino acids lysine, phenylalanine and
22 threonine were added to final concentrations of 100
23 mg l⁻¹ and isoleucine, leucine and valine to
24 50 mg l⁻¹. Seleno-L-methionine was added to a
25 concentration of 60 mg l⁻¹. The temperature was
26 lowered to 303 K and the culture left to shake for
27 further 15 min before protein overexpression was
28 induced with 1 mM IPTG. After 6 h cells were
29 harvested and lysed as described above. 13 mg pure
30 protein per litre of culture could be isolated.

1

2 **Protein analysis**

3

4 Following the two HPLC steps, the protein appeared to
5 be pure as judged by a SDS silver nitrate stained gel
6 (single band at an apparent molecular weight of 34
7 kDa); the calculated molecular weight based on
8 sequence being 33773 Da. A single peak with a
9 molecular weight of 33803 Da was found in the MALDI
10 mass spectrum. Dynamic light-scattering results
11 (DynaPro 801) indicated the native protein to be
12 monodisperse with a molecular weight in the range of
13 106 to 122 kDa indicative of a trimeric or tetrameric
14 protein. N-terminal sequencing was performed and
15 confirmed the protein to be RmlA.

16

17 The efficiency of the selenomethionine labelling
18 procedure was scrutinised by MALDI mass spectrometry.
19 A shift of +304 Da was found for the intact labelled
20 protein corresponding well to the predicted
21 additional mass of 282 Da (6 methionine residues per
22 chain). In an important and useful second check,
23 sulfur methionine containing fragments were
24 undetectable in the MALDI mass spectrum of a tryptic
25 protein digest.

26

27 **RmlA crystallisation**

28

29 Initial crystallisation conditions were obtained from
30 Screen I and II of Hampton Research (Jancarik & Kim,
31 1991; Cudney et al., 1994) plus NaCl, PEG 6000, PEG

1 6000/lithium sulphate and MPD grids. The sitting
2 drop vapour diffusion method (Ducruix & Giegé, 1992)
3 with 4 μ l of protein sample and 4 μ l of precipitant
4 at 293 K was used throughout. Crystals appeared
5 under 27 of the initial 192 conditions, in some cases
6 10 min after setup. Most promising were results from
7 the PEG 6000/lithium sulphate grid and hence these
8 conditions were further optimised. Plate type
9 crystals of approx. 0.3 x 0.3 x 0.05 mm size (Figure
10 2) were obtained after one to seven days using 9 to
11 12 % (w/v) PEG 6000, 0.5 M lithium sulphate and 0.1 M
12 citrate/NaOH pH 4.6 as precipitating solution. The
13 initial very high mosaicity of these crystals could
14 be greatly reduced by the addition of 1 to 2 μ l 10 to
15 50 mM G1P, dTMP or dTDP-glucose to the protein prior
16 to crystallisation.

17 18 Data collection

19
20 A 2.2 Å resolution dataset (see Table 1, Figure 4)
21 from a single flash frozen crystal grown in the
22 presence of G1P was collected in-house at 110 K using
23 a Nonius/MacScience DIP2000 imaging plate detector
24 system. Data were recorded as 245 non-overlapping 20
25 min 1° oscillations. Cryoprotection was achieved by
26 washing the crystal in mother liquor supplemented
27 with 16 % (v/v) PEG 600 for 10 to 15 s. The
28 oscillation images were indexed and integrated with
29 the program MOSFLM (Leslie, 1992) and scaled with the
30 CCP4 program SCALA (CCP4, 1994). Higher resolution
31 datasets of crystals grown in the presence of G1P,

1 dTMP, dTDP-glucose or thymidine/glucose-1-
2 phosphate/ AlF_3 were measured at the ESRF-Grenoble at
3 beamlines ID14EH1 and BM14 (Table 1). All crystals
4 were triclinic with approximate cell parameters of a
5 $= 71 \text{ \AA}$, $b = 73 \text{ \AA}$, $c = 134 \text{ \AA}$; $\alpha = 89.9^\circ$, $\beta = 81^\circ$ and γ
6 $= 81^\circ$. All attempts to index or reduce the data in a
7 higher spacegroup failed, a native Patterson map
8 shows no non-origin peak. A majority of the crystals
9 were actually twinned. This could only be detected
10 from the diffraction pattern. Trial and error was
11 used to locate single crystals for analysis. Flash-
12 annealing with the crystal remaining in the loop (Yeh
13 & Hol, 1998) in some cases helped to achieve a less
14 mosaic diffraction pattern.

15
16 In addition to the datasets shown in Table 1 (figure
17 4) a three-wavelength MAD experiment with a
18 selenomethionine labelled crystal that was grown in
19 the presence of GlP was carried out at beamline BM14
20 of the ESRF-Grenoble. The crystal-to-detector
21 distance was adjusted so that the outer rim of the
22 detector area corresponded to a resolution of 2.8 \AA .
23 730 non-overlapping 0.5° oscillations were recorded
24 at each of three wavelengths. The three wavelengths
25 were chosen from an EXAFS scan of the crystal to
26 correspond to the maximum of f'' (peak), the maximum
27 modulus of f' (inflection) and minimum modulus of f'
28 (remote). These data were indexed and integrated
29 with DENZO and scaled with SCALEPACK (Otwinowski &
30 Minor, 1996) and are shown in Table 2 (figure 5).

31

1 Preliminary structural characterisation

2

3 At the beginning of this study it was not clear
4 whether native RmlA is a trimeric or a tetrameric
5 protein. A self-rotation search of the TMP dataset
6 with REPLACE (Tong & Rossmann, 1997) reveals three
7 major ($> 30 \sigma$) plus several minor (approx. 10 to 15
8 σ) twofold axes (Figure 3). In addition, a 60° - and
9 a 120° -rotation axis (15.4 and 14.6 σ) are found
10 lying parallel to the major 180° -rotation axes at $\phi =$
11 8° and $\psi = 98^\circ$ (data not shown). The interpretation
12 of these results was greatly aided by the
13 determination of selenium atom positions with the
14 program SOLVE 1.17 (Terwilliger & Berentzen, 1999).
15 Twenty-four sites were found which could easily be
16 grouped into eight equivalent clusters of three
17 atoms. The clusters fall into two sets of four
18 indicating that RmlA is a tetramer and that the unit
19 cell of the P1 crystal form contains two tetrameric
20 molecules. The rotation superimposing the two
21 tetramers can be described as either as a 60° -, a
22 120° - or a 180° -rotation axis depending on which
23 monomer is used as a reference point. This explains
24 the existence of major and minor twofold axes in the
25 $\kappa=180^\circ$ self-rotation search. First, there are inter-
26 and intra-tetramer 180° -axes lying parallel to each
27 other. Second, in the case of exclusively intra-
28 tetramer axes only two pairs of two monomers are
29 superimposed while in the other the intramolecular
30 vectors of eight protein chains contribute to the

1 peak in the self rotation function, leading to a
2 stronger signal.

3

4 The asymmetric unit of the crystal contains
5 approximately 2400 amino acid residues and has a
6 solvent content of 51 %, corresponding to a V_M of
7 $2.54 \text{ \AA}^3 \text{ Da}^{-1}$ (Matthews, 1968).

8

9 A partial set of co-ordinates from *Pseudomonas*
10 *aeruginosa* RmlA is listed in Annex 1. The co-
11 ordinates are given in two sections; the first
12 section gives all atoms up to a distance of 15 Å to
13 the bound product in the active site; and the second
14 section gives all atoms up to a distance of 15 Å to
15 the bound product in the regulatory site. The data
16 is derived from the dTDP-glucose dataset given in
17 Figure 4 (table 1) and represent a model of excellent
18 geometrical properties with an R-factor of 16.3% and
19 an R_{free} of 21.8% at a resolution of 1.77 Å. The co-
20 ordinates also contain one bound molecule of dTDP-
21 glucose in each monomer's active centre, which can be
22 used in computer programs for inhibitor modelling.

23

24 STRUCTURAL CHARACTERISTICS

25

26 Fold

27

28 RmlA is a 222 tetrameric molecule and its structure
29 is represented in Fig. 6. In *Pseudomonas aeruginosa*
30 the monomer has a chain length of 293 amino acids.
31 The subunit's fold can be described as a single

1 domain $\alpha\beta\alpha$ sandwich, meaning that a central β -sheet
2 is covered by layers of helices from both sides. In
3 RmlA this mixed β -sheet is seven stranded in the
4 order 3214657 with strand 6 being antiparallel to the
5 rest. In addition, both helical layers contain a two
6 stranded β -sheet structure as well. Due to its
7 tetrameric nature each monomer is in contact with two
8 neighbouring subunits.

9 10 **Binding Sites**

11
12 The RmlA monomer is capable of binding two molecules
13 of dTDP-Glc. By sequence comparison with related
14 nucleotidyltransferases and inspection of the glucose
15 1-phosphate co-complex, it is possible to
16 definitively assign the active centre to the areas
17 around the black bound molecules in Fig. 6. The
18 second binding site (light grey molecules in Fig. 6)
19 is likely going to be involved in allosteric
20 regulation of RmlA's enzymic activity.

21 22 **Active Site**

23
24 The active site is exclusively made up of amino acids
25 from one monomer. Fig. 7 gives a schematic
26 representation of the most important interactions
27 between dTDP-Glc and the enzyme. The amino acids can
28 be subdivided into three groups.
29
30 Group one contains the residues involved in the
31 catalytic mechanism and in particular the formation

1 or pyrophosphorolysis of diphospho ester bonds.
2 Their importance is highlighted by a high degree of
3 conservation amongst nucleotidyltransferases. These
4 residues are Arg15, Asp110, Lys162 and Asp225. A
5 high degree of conservation is also observed for
6 Lys25 (not shown in Fig. 7). The positively charged
7 Arg15 and Lys25 are responsible of binding the β - and
8 the γ -phosphate group of dTDP as can be concluded
9 from an additional sulphate molecule that is bound in
10 the active site of RmlA but not shown in Figure 7.
11 The position of Lys25 is stabilised by a salt bridge
12 with Asp110, another highly conserved residue in
13 sugar nucleotidyltransferases. The importance of
14 Lys162 in the active centre lies in binding of the
15 phosphate group of glucose-1-phosphate. It ensures
16 correct orientation towards dTTP for nucleophilic
17 attack on the α -phosphate group.

18
19 Groups 2 and 3 provide specificity for thymidyl
20 and/or glucosyl ligands, respectively. Specificity
21 for the thymidyl moiety results from Gly10, Gln82 and
22 Gly87 which all form hydrogen bonds with the
23 pyrimidine ring. The glucose part of RmlA substrates
24 is hydrogen bonded to Asn111, Gly146, Glu161, Val172
25 and Tyr176. Among these, the chelating interaction
26 of Glu161's side chain will be of high importance as
27 it can only bind to hydroxyl groups of the sugar if
28 these are in equatorial position.

29
30 A hydrophobic patch of three leucine residues (Leu8,
31 Leu88, Leu108) lines the active site from the bottom.

1 Other residues in only hydrophobic interaction are
2 Pro85, Tyr145 and Trp223.
3
4
5

6 **Regulatory Site**

7

8 The second binding site for dTDP-Glc is located in
9 the interface between two monomers (Fig. 6), hence
10 amino acids from two subunits contribute to its
11 formation. The residues in this binding site (Fig.
12 8) are not conserved in more distantly related
13 nucleotidyltransferases. Therefore, these enzymes'
14 allosteric control might be achieved by other
15 mechanisms. However, glucose-1-phosphate
16 thymidyltransferases from other organisms will have
17 binding sites similar to Fig. 8 as can be concluded
18 from their amino acid sequences. It can be concluded
19 from Fig. 8 that dTDP-Glc is not the natural ligand
20 of this binding site as most contacts between the
21 protein and the glucosyl moiety are mediated by water
22 molecules whilst the remainder of the ligand shows
23 mainly direct hydrogen bonding.

24 Suitable inhibitors may either bind to the active
25 site of RmlA, acting in a competitive mode to natural
26 substrates and being non-cleavable, or may exploit
27 the allosteric properties of RmlA. In the case of
28 RmlA from *Pseudomonas aeruginosa* the latter might be
29 the preferred approach: the protein is strongly
30 inhibited by dTDP-rhamnose, the final product of the
31 four enzyme pathway (Melo & Glaser, 1965), possibly

1 by binding to the second binding site indicated in
2 Figure 6. As rhamnose is not found in mammals, dTDP-
3 rhamnose derived compounds might provide lesser side
4 effects in the application as antibiotics and are
5 potentially good candidates as suitable RmlA
6 inhibitors.

7
8 Several methods for assaying the activity of RmlA and
9 related enzymes in both sugar nucleotide synthesis
10 and pyrophosphorolysis directions have been described
11 in the literature. They are normally based on the
12 incorporation of radioactive compounds into the
13 reaction products and seem to be less suited for the
14 development of new inhibitors by high throughput
15 screening as they require a time-consuming separation
16 of the reaction mixtures. Therefore, it is proposed
17 to use coupled enzyme assays for drug development
18 purposes.

19
20 In the synthesis direction, the reaction can be
21 followed by monitoring the production of
22 pyrophosphate using pyrophosphate dependent fructose-
23 6-phosphate kinase (PP_i -PFK). This enzyme generates
24 fructose-1,6-diphosphate (F-1,6-DP) from fructose-6-
25 phosphate (F-6-P) and pyrophosphate (PP_i). F-1,6-DP
26 is then cleaved by aldolase to yield glyceraldehyde-
27 3-phosphate (GAP) and dihydroxyacetone phosphate
28 (DHAP). GAP is isomerised by triosephosphate
29 isomerase (TPI) to give a second molecule of DHAP.
30 Finally, DHAP is reduced to glycerol-3-phosphate
31 (G3P) by glycerophosphate dehydrogenase (GDH) in an

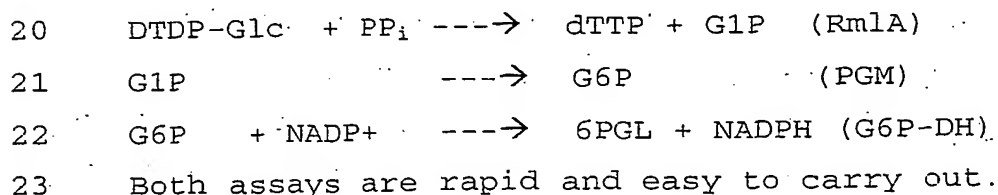
1 NADH-dependent reaction such that the production of
 2 pyrophosphate is coupled to the depletion of NADH
 3 which can be recorded by the decrease in absorption
 4 at 340 nm (O'Brien, 1976):



10

11 The pyrophosphorolysis direction can be monitored by
 12 following the production of G1P, which is then
 13 isomerised to glucose-6-phosphate by
 14 phosphoglucomutase (PGM) and subsequently oxidised to
 15 6-phospho-gluconolactone (6PGL) by glucose-6-
 16 phosphate dehydrogenase (G6P-DH), thereby generating
 17 one molecule of NADPH. This can again be followed at
 18 340 nm (Kornfeld & Glaser, 1961):

19



24

25 The active and regulatory sites of RmlA and
 26 interactions with their natural substrates are
 27 further illustrated by the Figures...

28

29

30

31

Annex 1 : 22

REGULATORY SITES

REMARK Created by MOLEMAN2 V. 990504/2.3 at Thu Jul 13 16:59:55 2000 for wulf

REMARK 3

REMARK 3 REFINEMENT.

REMARK 3 PROGRAM : REFMAC

REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON

REMARK 3

REMARK 3 Maximum likelihood refinement was used

REMARK 3

REMARK 3 DATA USED IN REFINEMENT.

REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.7

REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 73.

REMARK 3 DATA CUTOFF (SIGMA(F)) : 0.0

REMARK 3 COMPLETENESS FOR RANGE (%) : 82.7

REMARK 3 NUMBER OF REFLECTIONS : 230146

REMARK 3

REMARK 3 FIT TO DATA USED IN REFINEMENT.

REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT

REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM

REMARK 3 R VALUE (WORKING + TEST SET) : 0.16587

REMARK 3 R VALUE (WORKING SET) : 0.16312

REMARK 3 FREE R VALUE : 0.21818

REMARK 3 FREE R VALUE TEST SET SIZE (%) : 5.0

REMARK 3 FREE R VALUE TEST SET COUNT : 12192

REMARK 3

REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.

REMARK 3 All atoms : 46517

REMARK 3

REMARK 3 B VALUES.

REMARK 3 FROM WILSON PLOT (A**2) : NULL

REMARK 3 MEAN B VALUE (OVERALL, A**2) : 14.387

REMARK 3 OVERALL ANISOTROPIC B VALUE.

REMARK 3 B11 (A**2) : 0.46

REMARK 3 B22 (A**2) : -0.19

REMARK 3 B33 (A**2) : -0.27

REMARK 3 B12 (A**2) : 0.03

REMARK 3 B13 (A**2) : -0.02

REMARK 3 B23 (A**2) : -0.25

REMARK 3

REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.

REMARK 3 ESU BASED ON R VALUE (A):

REMARK 3 NULL

REMARK 3 ESU BASED ON FREE R VALUE (A):

REMARK 3 0.18277

REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD (A):

REMARK 3 0.12940

REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):

REMARK 3 8.01924

REMARK 3

REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.

REMARK 3 DISTANCE RESTRAINTS. RMS SIGMA

REMARK 3 BOND LENGTH (A) : 0.021 ; 0.021

REMARK 3 BOND ANGLE (DEGREES) : 2.076 ; 2.015

REMARK 3 Torsion angles, period 1 (DEGREES) : 5.103 ; 3.000

REMARK 3 Torsion angles, period 3 (DEGREES) : 16.457 ; 15.000

REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3) : 0.126 ; 0.200

REMARK 3 PLANE RESTRAINT (A) : 0.009 ; 0.020

REMARK 3 VDW repulsions (A) : 0.232 ; 0.300

REMARK 3 Potential hbonds (A) : 0.217 ; 0.500

REMARK 3

REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA

REMARK 3 MAIN-CHAIN BOND (A**2) : 1.443 ; 1.500

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REMARK 3 MAIN-CHAIN ANGLE (A**2) : 2.158 ; 2.000
REMARK 3 SIDE-CHAIN BOND (A**2) : 3.125 ; 3.000
REMARK 3 SIDE-CHAIN ANGLE (A**2) : 4.584 ; 4.500
REMARK 3
REMARK 3 ANISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 Rigid-bond restraints (A**2) : 1.894 ; 2.000
REMARK 3 Sphericity; free atoms (A**2) : 4.664 ; 2.000
REMARK 3 Sphericity; bonded atoms (A**2) : 2.553 ; 2.000
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS.
REMARK 3
REMARK 3 TLS details
REMARK 3 Number of tls groups : 8
REMARK 3
REMARK 3 Number of pieces in the TLS group 1: 1
REMARK 3 From A 1 to A 292
REMARK 3 Origin for the group : 1
REMARK 3 69.4830 59.4220 78.9970
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0325 0.0433 0.0247 -0.0039 -0.0136 -0.0012
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6102 0.6435 0.4229 -0.1271 0.0884 -0.0867
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 0.0248 -0.0135 -0.0505 0.0232 0.0615 -0.0461 0.0207 -0.0758
REMARK 3
REMARK 3 Number of pieces in the TLS group 2: 1
REMARK 3 From B 1 to B 293
REMARK 3 Origin for the group : 2
REMARK 3 61.2650 33.4890 54.1360
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0294 0.0510 0.0183 0.0014 0.0082 -0.0045
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6794 0.6303 0.4419 0.1224 -0.1618 -0.1218
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0046 -0.0119 0.0109 0.0234 0.0528 0.0423 -0.0173 -0.0642
REMARK 3
REMARK 3 Number of pieces in the TLS group 3: 1
REMARK 3 From C 1 to C 292
REMARK 3 Origin for the group : 3
REMARK 3 100.4020 45.2900 79.2890
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0309 0.0357 0.0395 0.0126 0.0217 0.0172
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.5756 0.7497 0.6477 -0.1840 0.0581 -0.3103
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0999 -0.0112 0.0060 0.0283 -0.1071 -0.0800 0.0406 0.0887
REMARK 3
REMARK 3 Number of pieces in the TLS group 4: 1
REMARK 3 From D 1 to D 292
REMARK 3 Origin for the group : 4
REMARK 3 93.1810 38.1690 43.3930
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0110 0.0453 0.0536 0.0109 0.0225 0.0295
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6426 0.7184 0.8911 0.0882 -0.0950 -0.4089
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.1237 -0.0615 0.0018 -0.0411 -0.1339 -0.0574 0.0193 0.1369
REMARK 3
REMARK 3 Number of pieces in the TLS group 5: 1
REMARK 3 From E 1 to E 292
REMARK 3 Origin for the group : 5

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```

REMARK 3 42.8770 8.9030 19.5730
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0309 0.0452 0.0352 0.0089 -0.0125 -0.0200
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6312 0.7631 0.9845 0.0814 0.0288 0.4970
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.1195 -0.0434 -0.0468 0.0342 0.1311 -0.0463 -0.0408 -0.1559
REMARK 3
REMARK 3 Number of pieces in the TLS group 6: 1
REMARK 3 From F 1 to F 293
REMARK 3 Origin for the group : 6
REMARK 3 38.0920 17.7800 -16.3490
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0208 0.0425 0.0417 0.0034 0.0045 -0.0015
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.8800 0.3582 0.6933 0.1180 0.1354 0.1904
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0810 0.0464 -0.0329 0.0291 0.0416 0.0160 -0.0440 -0.0740
REMARK 3
REMARK 3 Number of pieces in the TLS group 7: 1
REMARK 3 From G 1 to G 292
REMARK 3 Origin for the group : 7
REMARK 3 71.8950 21.8640 -15.9250
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0234 0.0522 0.0272 -0.0024 -0.0109 0.0094
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.5696 0.5742 0.4250 0.0699 -0.0286 -0.0019
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0333 0.0146 0.0152 -0.0110 -0.0283 0.0204 -0.0007 0.0589
REMARK 3
REMARK 3 Number of pieces in the TLS group 8: 1
REMARK 3 From H 1 to H 292
REMARK 3 Origin for the group : 8
REMARK 3 71.9070 -5.2410 8.8240
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0445 0.0386 0.0064 0.0038 0.0132 0.0109
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.4837 0.7743 0.6523 -0.1036 -0.1161 0.0699
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0109 -0.0288 -0.0166 0.0049 -0.0575 -0.0486 0.0096 0.0981
REMARK 3
REMARK 3 Hydrogens have been added in the riding positions
REMARK 3
REMARK 3
REMARK 3 Scaling details
REMARK 3 Babinet"s principle for scaling has been used
REMARK 3 Bulk solvent correction based on constant value has been used
REMARK 3 Parameters for mask calculation
REMARK 3 VDW prob radii = 1.40
REMARK 3 ION prob radii = 0.80
REMARK 3 Shrinkage radii = 0.80
REMARK 3
HEADER ---- XX-XXX-XX xxxx
COMPND ---
CISPEP 1 HIS A 16 PRO A 17 0.00
CISPEP 2 HIS B 17 PRO B 18 0.00
CISPEP 3 HIS C 16 PRO C 17 0.00
CISPEP 4 HIS D 16 PRO D 17 0.00
CISPEP 5 HIS E 16 PRO E 17 0.00
CISPEP 6 HIS G 16 PRO G 17 0.00
CISPEP 7 HIS H 16 PRO H 17 0.00

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CISPEP	8	HIS	F	17	PRO	F	18				0.00							
CRYST1	71.575			73.410			134.290	89.94	80.61	80.93	P 1						1	
ORIGX1				1.000000			0.000000	0.000000			0.000000							
ORIGX2				0.000000			1.000000	0.000000			0.000000							
ORIGX3				0.000000			0.000000	1.000000			0.000000							
SCALE1				0.013971			-0.002230	-0.002368			0.000000							
SCALE2				0.000000			0.013795	0.000349			0.000000							
SCALE3				0.000000			0.000000	0.007550			0.000000							
ATOM	6294	C	LEU	B	112			68.475	34.973	54.827	1.00	9.88						C
ANISOU	6294	C	LEU	B	112			1175	1368	1209	75	80					2	C
ATOM	6295	O	LEU	B	112			69.411	34.350	55.217	1.00	11.66						O
ANISOU	6295	O	LEU	B	112			1490	1423	1514	112	11					82	O
ATOM	6296	N	TYR	B	113			68.162	35.030	53.563	1.00	9.61						N
ANISOU	6296	N	TYR	B	113			1127	1258	1266	59	42					-9	N
ATOM	6298	CA	TYR	B	113			68.953	34.395	52.503	1.00	7.80						C
ANISOU	6298	CA	TYR	B	113			999	1040	923	4	94					26	C
ATOM	6300	CB	TYR	B	113			68.065	33.564	51.581	1.00	7.86						C
ANISOU	6300	CB	TYR	B	113			1027	1071	886	7	152					26	C
ATOM	6303	CG	TYR	B	113			67.339	32.444	52.224	1.00	9.60						C
ANISOU	6303	CG	TYR	B	113			1325	1269	1053	-43	-63					29	C
ATOM	6304	CD1	TYR	B	113			66.069	32.627	52.749	1.00	11.51						C
ANISOU	6304	CD1	TYR	B	113			1341	1555	1476	-4	99					21	C
ATOM	6306	CE1	TYR	B	113			65.378	31.548	53.357	1.00	10.21						C
ANISOU	6306	CE1	TYR	B	113			1180	1285	1413	23	46					8	C
ATOM	6308	CZ	TYR	B	113			65.973	30.311	53.427	1.00	11.84						C
ANISOU	6308	CZ	TYR	B	113			1573	1440	1484	-3	84					54	C
ATOM	6309	OH	TYR	B	113			65.307	29.256	54.015	1.00	10.12						O
ANISOU	6309	OH	TYR	B	113			946	1215	1681	158	-103					326	O
ATOM	6311	CE2	TYR	B	113			67.183	30.109	52.837	1.00	11.43						C
ANISOU	6311	CE2	TYR	B	113			1157	1317	1868	72	-151					158	C
ATOM	6313	CD2	TYR	B	113			67.860	31.177	52.211	1.00	10.78						C
ANISOU	6313	CD2	TYR	B	113			1431	1394	1271	115	-249					126	C
ATOM	6315	C	TYR	B	113			69.639	35.484	51.642	1.00	7.73						C
ANISOU	6315	C	TYR	B	113			1030	1027	878	43	56					33	C
ATOM	6316	O	TYR	B	113			69.122	36.576	51.488	1.00	7.43						O
ANISOU	6316	O	TYR	B	113			1163	1019	639	56	111					197	O
ATOM	6317	N	TYR	B	114			70.843	35.209	51.135	1.00	7.30						N
ANISOU	6317	N	TYR	B	114			1038	916	817	78	37					-24	N
ATOM	6319	CA	TYR	B	114			71.408	36.134	50.234	1.00	7.79						C
ANISOU	6319	CA	TYR	B	114			882	1085	990	69	20					22	C
ATOM	6321	CB	TYR	B	114			72.075	37.313	50.967	1.00	8.84						C
ANISOU	6321	CB	TYR	B	114			1069	1172	1115	76	64					44	C
ATOM	6324	CG	TYR	B	114			72.428	38.431	50.016	1.00	9.10						C
ANISOU	6324	CG	TYR	B	114			1248	1039	1167	-28	-201					-16	C
ATOM	6325	CD1	TYR	B	114			71.472	39.349	49.662	1.00	11.13						C
ANISOU	6325	CD1	TYR	B	114			1300	1304	1623	182	38					12	C
ATOM	6327	CE1	TYR	B	114			71.757	40.357	48.767	1.00	10.49						C
ANISOU	6327	CE1	TYR	B	114			1484	1042	1460	33	-6					56	C
ATOM	6329	CZ	TYR	B	114			73.027	40.460	48.216	1.00	10.67						C
ANISOU	6329	CZ	TYR	B	114			1385	1305	1363	41	-167					37	C
ATOM	6330	OH	TYR	B	114			73.311	41.487	47.315	1.00	11.18						O
ANISOU	6330	OH	TYR	B	114			1336	1359	1553	-239	-299					48	O
ATOM	6332	CE2	TYR	B	114			74.011	39.546	48.570	1.00	7.62						C
ANISOU	6332	CE2	TYR	B	114			1062	898	935	-44	-259					-116	C
ATOM	6334	CD2	TYR	B	114			73.694	38.559	49.478	1.00	7.95						C
ANISOU	6334	CD2	TYR	B	114			1246	731	1040	-6	-52					-122	C
ATOM	6336	C	TYR	B	114			72.432	35.447	49.350	1.00	9.28						C
ANISOU	6336	C	TYR	B	114			1204	1240	1080	131	53					41	C
ATOM	6337	O	TYR	B	114			73.302	34.666	49.833	1.00	8.68						O
ANISOU	6337	O	TYR	B	114			789	1307	1201	372	113					51	O
ATOM	6338	N	GLY	B	115			72.434	35.845	48.090	1.00	8.73						N

ANISOU	6338	N	GLY	B	115	1039	1276	1000	84	-100	32	N
ATOM	6340	CA	GLY	B	115	73.544	35.449	47.224	1.00	8.72		C
ANISOU	6340	CA	GLY	B	115	1098	1144	1070	109	57	82	C
ATOM	6343	C	GLY	B	115	73.295	35.510	45.744	1.00	7.38		C
ANISOU	6343	C	GLY	B	115	896	921	985	-61	0	30	C
ATOM	6344	O	GLY	B	115	72.171	35.797	45.261	1.00	9.26		O
ANISOU	6344	O	GLY	B	115	1156	1243	1119	112	-74	144	O
ATOM	6345	N	HIS	B	116	74.349	35.220	45.007	1.00	7.30		N
ANISOU	6345	N	HIS	B	116	932	922	917	44	-5	-10	N
ATOM	6347	CA	HIS	B	116	74.300	35.259	43.540	1.00	7.38		C
ANISOU	6347	CA	HIS	B	116	923	986	893	104	-25	85	C
ATOM	6349	CB	HIS	B	116	75.727	35.106	42.945	1.00	7.55		C
ANISOU	6349	CB	HIS	B	116	1013	928	928	55	10	103	C
ATOM	6352	CG	HIS	B	116	75.746	35.098	41.450	1.00	8.35		C
ANISOU	6352	CG	HIS	B	116	1105	1070	996	10	41	38	C
ATOM	6353	ND1	HIS	B	116	75.393	36.207	40.714	1.00	8.46		N
ANISOU	6353	ND1	HIS	B	116	1206	1073	932	121	83	126	N
ATOM	6355	CE1	HIS	B	116	75.484	35.904	39.425	1.00	11.58		C
ANISOU	6355	CE1	HIS	B	116	1633	1464	1302	-142	-36	4	C
ATOM	6357	NE2	HIS	B	116	76.029	34.697	39.306	1.00	11.15		N
ANISOU	6357	NE2	HIS	B	116	1161	1704	1369	-4	4	75	N
ATOM	6359	CD2	HIS	B	116	76.164	34.156	40.561	1.00	9.33		C
ANISOU	6359	CD2	HIS	B	116	1144	1203	1198	69	-66	14	C
ATOM	6361	C	HIS	B	116	73.386	34.229	42.935	1.00	8.57		C
ANISOU	6361	C	HIS	B	116	1024	1176	1055	73	-18	97	C
ATOM	6362	O	HIS	B	116	73.424	33.059	43.290	1.00	7.60		O
ANISOU	6362	O	HIS	B	116	834	952	1099	171	-185	110	O
ATOM	6363	N	ASP	B	117	72.503	34.689	42.016	1.00	8.98		N
ANISOU	6363	N	ASP	B	117	1046	1282	1081	86	-30	101	N
ATOM	6365	CA	ASP	B	117	71.577	33.796	41.357	1.00	10.33		C
ANISOU	6365	CA	ASP	B	117	1230	1401	1293	75	-56	22	C
ATOM	6367	CB	ASP	B	117	72.288	32.804	40.432	1.00	10.54		C
ANISOU	6367	CB	ASP	B	117	1223	1471	1309	-39	-37	57	C
ATOM	6370	CG	ASP	B	117	72.760	33.467	39.144	1.00	13.93		C
ANISOU	6370	CG	ASP	B	117	1930	1747	1614	-23	86	51	C
ATOM	6371	OD1	ASP	B	117	72.736	34.739	39.047	1.00	14.18		O
ANISOU	6371	OD1	ASP	B	117	1749	1876	1759	63	54	40	O
ATOM	6372	OD2	ASP	B	117	73.128	32.765	38.171	1.00	14.50		O
ANISOU	6372	OD2	ASP	B	117	2369	1619	1519	-153	438	256	O
ATOM	6373	C	ASP	B	117	70.566	33.127	42.295	1.00	10.52		C
ANISOU	6373	C	ASP	B	117	1403	1334	1258	40	-96	70	C
ATOM	6374	O	ASP	B	117	69.981	32.125	41.968	1.00	11.35		O
ANISOU	6374	O	ASP	B	117	1603	1565	1142	-22	-206	-145	O
ATOM	6375	N	PHE	B	118	70.325	33.724	43.461	1.00	10.07		N
ANISOU	6375	N	PHE	B	118	1330	1308	1188	19	-23	-15	N
ATOM	6377	CA	PHE	B	118	69.265	33.250	44.360	1.00	10.62		C
ANISOU	6377	CA	PHE	B	118	1337	1348	1347	-56	-20	30	C
ATOM	6379	CB	PHE	B	118	69.265	34.048	45.664	1.00	9.09		C
ANISOU	6379	CB	PHE	B	118	1034	1158	1259	-117	21	-26	C
ATOM	6382	CG	PHE	B	118	68.298	33.591	46.684	1.00	9.98		C
ANISOU	6382	CG	PHE	B	118	1369	1144	1277	25	49	-41	C
ATOM	6383	CD1	PHE	B	118	68.327	32.317	47.151	1.00	11.71		C
ANISOU	6383	CD1	PHE	B	118	1659	1400	1388	23	178	61	C
ATOM	6385	CE1	PHE	B	118	67.478	31.934	48.165	1.00	10.86		C
ANISOU	6385	CE1	PHE	B	118	1297	1145	1683	-313	161	-107	C
ATOM	6387	CZ	PHE	B	118	66.568	32.812	48.671	1.00	11.10		C
ANISOU	6387	CZ	PHE	B	118	1255	1529	1430	-14	159	112	C
ATOM	6389	CE2	PHE	B	118	66.565	34.096	48.281	1.00	8.70		C
ANISOU	6389	CE2	PHE	B	118	957	1364	982	81	60	-100	C
ATOM	6391	CD2	PHE	B	118	67.419	34.500	47.291	1.00	10.35		C
ANISOU	6391	CD2	PHE	B	118	951	1393	1588	-123	128	124	C

ATOM	6393	C	PHE B 118	67.899	33.376	43.636	1.00	11.03				C
ANISOU	6393	C	PHE B 118	1376	1421	1391	11	27	-19			C
ATOM	6394	O	PHE B 118	67.010	32.543	43.766	1.00	8.89				O
ANISOU	6394	O	PHE B 118	1283	924	1170	-61	1	13			O
ATOM	6395	N	HIS B 119	67.774	34.420	42.847	1.00	10.46				N
ANISOU	6395	N	HIS B 119	1382	1248	1343	5	51	62			N
ATOM	6397	CA	HIS B 119	66.552	34.600	42.091	1.00	12.15				C
ANISOU	6397	CA	HIS B 119	1573	1523	1517	-14	-27	-40			C
ATOM	6399	CB	HIS B 119	66.557	35.954	41.401	1.00	12.68				C
ANISOU	6399	CB	HIS B 119	1620	1448	1749	41	32	-109			C
ATOM	6402	CG	HIS B 119	66.889	35.944	39.972	1.00	18.70				C
ANISOU	6402	CG	HIS B 119	2504	2437	2162	-139	42	8			C
ATOM	6403	ND1	HIS B 119	67.827	36.827	39.463	1.00	22.72				N
ANISOU	6403	ND1	HIS B 119	2685	3073	2872	-225	-65	26			N
ATOM	6411	C	HIS B 119	66.193	33.405	41.166	1.00	11.61				C
ANISOU	6411	C	HIS B 119	1547	1433	1429	9	-35	41			C
ATOM	6412	O	HIS B 119	65.043	32.995	41.111	1.00	11.02				O
ANISOU	6412	O	HIS B 119	1259	1530	1395	94	-68	68			O
ATOM	6413	N	GLU B 120	67.174	32.888	40.461	1.00	10.93				N
ANISOU	6413	N	GLU B 120	1467	1471	1214	25	-66	6			N
ATOM	6415	CA	GLU B 120	66.991	31.725	39.622	1.00	11.64				C
ANISOU	6415	CA	GLU B 120	1478	1482	1463	-39	-22	37			C
ATOM	6417	CB	GLU B 120	68.220	31.541	38.710	1.00	11.47				C
ANISOU	6417	CB	GLU B 120	1616	1367	1374	-5	34	-74			C
ATOM	6420	CG	GLU B 120	68.367	32.582	37.606	1.00	11.87				C
ANISOU	6420	CG	GLU B 120	1568	1419	1520	-17	-16	-24			C
ATOM	6423	CD	GLU B 120	69.184	33.815	37.959	1.00	12.06				C
ANISOU	6423	CD	GLU B 120	1560	1559	1461	-96	108	-68			C
ATOM	6424	OE1	GLU B 120	69.358	34.067	39.172	1.00	10.94				O
ANISOU	6424	OE1	GLU B 120	1081	1425	1649	-231	-268	-44			O
ATOM	6425	OE2	GLU B 120	69.633	34.517	36.994	1.00	12.75				O
ANISOU	6425	OE2	GLU B 120	1713	1273	1858	-323	48	124			O
ATOM	6426	C	GLU B 120	66.738	30.447	40.463	1.00	12.14				C
ANISOU	6426	C	GLU B 120	1553	1595	1462	-76	61	-6			C
ATOM	6427	O	GLU B 120	65.936	29.598	40.062	1.00	10.95				O
ANISOU	6427	O	GLU B 120	1296	1624	1237	-177	287	-89			O
ATOM	6428	N	LEU B 121	67.438	30.322	41.604	1.00	12.30				N
ANISOU	6428	N	LEU B 121	1528	1613	1529	-105	-32	42			N
ATOM	6430	CA	LEU B 121	67.249	29.199	42.539	1.00	12.52				C
ANISOU	6430	CA	LEU B 121	1544	1641	1571	-103	-13	26			C
ATOM	6432	CB	LEU B 121	68.151	29.344	43.765	1.00	12.80				C
ANISOU	6432	CB	LEU B 121	1525	1770	1568	-76	-14	20			C
ATOM	6435	CG	LEU B 121	68.175	28.110	44.725	1.00	15.74				C
ANISOU	6435	CG	LEU B 121	2079	1908	1991	-88	-70	80			C
ATOM	6437	CD1	LEU B 121	68.778	26.950	44.030	1.00	21.04				C
ANISOU	6437	CD1	LEU B 121	2605	2649	2737	82	-4	7			C
ATOM	6441	CD2	LEU B 121	68.933	28.316	46.002	1.00	14.06				C
ANISOU	6441	CD2	LEU B 121	1921	1916	1505	9	196	85			C
ATOM	6445	C	LEU B 121	65.777	29.186	42.987	1.00	10.89				C
ANISOU	6445	C	LEU B 121	1258	1424	1454	4	0	-22			C
ATOM	6446	O	LEU B 121	65.074	28.129	42.945	1.00	11.39				O
ANISOU	6446	O	LEU B 121	1244	1362	1719	-52	205	-2			O
ATOM	6447	N	LEU B 122	65.270	30.347	43.325	1.00	10.11				N
ANISOU	6447	N	LEU B 122	1206	1325	1308	-89	-42	-4			N
ATOM	6449	CA	LEU B 122	63.826	30.466	43.703	1.00	9.01				C
ANISOU	6449	CA	LEU B 122	1042	1213	1166	-10	8	79			C
ATOM	6451	CB	LEU B 122	63.576	31.857	44.218	1.00	8.22				C
ANISOU	6451	CB	LEU B 122	826	1242	1054	-142	37	45			C
ATOM	6454	CG	LEU B 122	64.227	32.253	45.565	1.00	8.65				C
ANISOU	6454	CG	LEU B 122	982	1247	1056	-1	188	-86			C
ATOM	6456	CD1	LEU B 122	64.051	33.713	45.823	1.00	9.74				C

ANISOU	6456	CD1	LEU	B	122	1117	1199	1382	104	50	169	C
ATOM	6460	CD2	LEU	B	122	63.707	31.467	46.720	1.00	9.31		C
ANISOU	6460	CD2	LEU	B	122	1313	1116	1108	-102	70	113	C
ATOM	6464	C	LEU	B	122	62.822	30.173	42.553	1.00	10.11		C
ANISOU	6464	C	LEU	B	122	1356	1175	1310	-111	68	-105	C
ATOM	6465	O	LEU	B	122	61.810	29.486	42.674	1.00	9.51		O
ANISOU	6465	O	LEU	B	122	832	1369	1411	-35	-12	-23	O
ATOM	6466	N	GLY	B	123	63.108	30.726	41.414	1.00	11.03		N
ANISOU	6466	N	GLY	B	123	1584	1342	1264	-123	41	-73	N
ATOM	6468	CA	GLY	B	123	62.290	30.499	40.249	1.00	12.07		C
ANISOU	6468	CA	GLY	B	123	1532	1575	1478	-125	29	-4	C
ATOM	6471	C	GLY	B	123	62.228	29.038	39.810	1.00	12.25		C
ANISOU	6471	C	GLY	B	123	1673	1559	1419	-73	26	41	C
ATOM	6472	O	GLY	B	123	61.135	28.604	39.406	1.00	13.28		O
ANISOU	6472	O	GLY	B	123	1625	1867	1553	-189	25	-20	O
ATOM	6473	N	SER	B	124	63.335	28.298	39.872	1.00	12.13		N
ANISOU	6473	N	SER	B	124	1435	1717	1456	-163	105	61	N
ATOM	6475	CA	SER	B	124	63.315	26.867	39.522	1.00	12.94		C
ANISOU	6475	CA	SER	B	124	1629	1762	1522	-36	34	36	C
ATOM	6477	CB	SER	B	124	64.666	26.237	39.634	1.00	13.63		C
ANISOU	6477	CB	SER	B	124	1712	1804	1662	-70	12	55	C
ATOM	6480	OG	SER	B	124	65.493	26.745	38.613	1.00	16.55		O
ANISOU	6480	OG	SER	B	124	2085	2182	2019	33	101	182	O
ATOM	6482	C	SER	B	124	62.375	26.135	40.476	1.00	13.37		C
ANISOU	6482	C	SER	B	124	1756	1776	1547	-167	33	42	C
ATOM	6483	O	SER	B	124	61.508	25.348	40.054	1.00	13.72		O
ANISOU	6483	O	SER	B	124	2075	1848	1290	-232	-85	-107	O
ATOM	6484	N	ALA	B	125	62.492	26.428	41.769	1.00	11.71		N
ANISOU	6484	N	ALA	B	125	1465	1587	1396	-135	5	-19	N
ATOM	6486	CA	ALA	B	125	61.581	25.745	42.713	1.00	11.64		C
ANISOU	6486	CA	ALA	B	125	1586	1505	1331	-105	15	1	C
ATOM	6488	CB	ALA	B	125	62.073	25.892	44.139	1.00	11.91		C
ANISOU	6488	CB	ALA	B	125	1558	1486	1479	-152	-17	-40	C
ATOM	6492	C	ALA	B	125	60.122	26.192	42.572	1.00	10.84		C
ANISOU	6492	C	ALA	B	125	1498	1387	1230	-84	5	11	C
ATOM	6532	CD	ARG	B	128	60.298	21.165	41.519	1.00	18.77		C
ANISOU	6532	CD	ARG	B	128	2511	2444	2177	-125	28	27	C
ATOM	6535	NE	ARG	B	128	61.529	20.700	40.936	1.00	21.99		N
ANISOU	6535	NE	ARG	B	128	2812	2583	2959	144	-310	-156	N
ATOM	6537	CZ	ARG	B	128	61.999	19.477	40.972	1.00	15.47		C
ANISOU	6537	CZ	ARG	B	128	2036	2102	1740	-116	-470	-99	C
ATOM	6538	NH1	ARG	B	128	61.420	18.557	41.653	1.00	14.38		N
ANISOU	6538	NH1	ARG	B	128	1712	2162	1589	-277	-394	56	N
ATOM	6541	NH2	ARG	B	128	63.111	19.242	40.373	1.00	17.94		N
ANISOU	6541	NH2	ARG	B	128	2299	2506	2010	-56	-175	-77	N
ATOM	6596	CA	SER	B	133	61.003	21.436	47.325	1.00	7.43		C
ANISOU	6596	CA	SER	B	133	863	1003	957	13	-60	-44	C
ATOM	6598	CB	SER	B	133	61.254	22.334	46.130	1.00	7.20		C
ANISOU	6598	CB	SER	B	133	722	952	1061	9	-42	-6	C
ATOM	6601	OG	SER	B	133	60.798	21.793	44.885	1.00	7.70		O
ANISOU	6601	OG	SER	B	133	713	1276	936	-69	-172	17	O
ATOM	6603	C	SER	B	133	61.483	22.145	48.596	1.00	7.62		C
ANISOU	6603	C	SER	B	133	986	957	950	14	48	-40	C
ATOM	6604	O	SER	B	133	60.831	23.068	49.081	1.00	8.09		O
ANISOU	6604	O	SER	B	133	941	1173	958	-58	192	-139	O
ATOM	6605	N	VAL	B	134	62.653	21.739	49.068	1.00	6.84		N
ANISOU	6605	N	VAL	B	134	804	875	916	48	102	-104	N
ATOM	6607	CA	VAL	B	134	63.297	22.261	50.256	1.00	6.93		C
ANISOU	6607	CA	VAL	B	134	868	930	834	19	-8	-46	C
ATOM	6609	CB	VAL	B	134	63.078	21.349	51.462	1.00	8.11		C
ANISOU	6609	CB	VAL	B	134	1060	1036	985	-19	65	-54	C

ATOM	6615	CG2	VAL	B	134	63.850	20.005	51.357	1.00	9.68	
ANISOU	6615	CG2	VAL	B	134	1360	1156	1158	-123	20	12
ATOM	6619	C	VAL	B	134	64.797	22.369	49.946	1.00	7.97	
ANISOU	6619	C	VAL	B	134	995	1003	1027	-43	0	-43
ATOM	6620	O	VAL	B	134	65.247	21.827	48.978	1.00	9.70	
ANISOU	6620	O	VAL	B	134	1066	1341	1278	-36	-109	-156
ATOM	6621	N	PHE	B	135	65.546	23.086	50.772	1.00	7.57	
ANISOU	6621	N	PHE	B	135	1017	1087	770	15	-49	-23
ATOM	6623	CA	PHE	B	135	66.943	23.426	50.530	1.00	8.09	
ANISOU	6623	CA	PHE	B	135	1012	1097	963	73	-29	1
ATOM	6625	CB	PHE	B	135	67.060	24.916	50.305	1.00	8.70	
ANISOU	6625	CB	PHE	B	135	832	1327	1146	-61	51	-8
ATOM	6628	CG	PHE	B	135	66.273	25.377	49.135	1.00	10.94	
ANISOU	6628	CG	PHE	B	135	1378	1321	1455	-61	-99	-36
ATOM	6629	CD1	PHE	B	135	64.942	25.787	49.294	1.00	14.22	
ANISOU	6629	CD1	PHE	B	135	1604	1903	1893	17	3	-14
ATOM	6631	CE1	PHE	B	135	64.203	26.127	48.196	1.00	16.39	
ANISOU	6631	CE1	PHE	B	135	1777	2233	2218	141	77	76
ATOM	6633	CZ	PHE	B	135	64.778	26.094	46.936	1.00	17.11	
ANISOU	6633	CZ	PHE	B	135	2309	2123	2068	20	-158	43
ATOM	6635	CE2	PHE	B	135	66.033	25.682	46.784	1.00	15.86	
ANISOU	6635	CE2	PHE	B	135	2082	2010	1932	-51	76	89
ATOM	6637	CD2	PHE	B	135	66.787	25.306	47.883	1.00	14.39	
ANISOU	6637	CD2	PHE	B	135	1818	1885	1763	-16	78	51
ATOM	6639	C	PHE	B	135	67.798	22.981	51.711	1.00	8.70	
ANISOU	6639	C	PHE	B	135	1170	1129	1004	46	-36	-35
ATOM	6640	O	PHE	B	135	67.394	23.171	52.873	1.00	9.72	
ANISOU	6640	O	PHE	B	135	1520	1230	940	-29	-39	247
ATOM	6641	N	ALA	B	136	68.910	22.321	51.386	1.00	7.74	
ANISOU	6641	N	ALA	B	136	892	1086	961	-16	-61	100
ATOM	6643	CA	ALA	B	136	69.870	21.847	52.388	1.00	7.69	
ANISOU	6643	CA	ALA	B	136	965	998	958	-3	-41	84
ATOM	6645	CB	ALA	B	136	70.215	20.419	52.076	1.00	8.30	
ANISOU	6645	CB	ALA	B	136	970	1226	956	17	-65	41
ATOM	6649	C	ALA	B	136	71.120	22.726	52.405	1.00	8.69	
ANISOU	6649	C	ALA	B	136	1163	1108	1030	-9	-2	55
ATOM	6650	O	ALA	B	136	71.699	23.024	51.348	1.00	9.88	
ANISOU	6650	O	ALA	B	136	1248	1395	1108	-236	212	50
ATOM	6651	N	TYR	B	137	71.562	23.103	53.600	1.00	7.61	
ANISOU	6651	N	TYR	B	137	1117	1021	750	-86	47	79
ATOM	6653	CA	TYR	B	137	72.668	24.023	53.761	1.00	7.01	
ANISOU	6653	CA	TYR	B	137	858	959	848	50	-29	4
ATOM	6655	CB	TYR	B	137	72.170	25.396	54.039	1.00	5.60	
ANISOU	6655	CB	TYR	B	137	660	986	481	158	64	-15
ATOM	6658	CG	TYR	B	137	73.094	26.593	54.050	1.00	7.74	
ANISOU	6658	CG	TYR	B	137	972	916	1050	145	-45	29
ATOM	6659	CD1	TYR	B	137	73.395	27.309	52.887	1.00	8.47	
ANISOU	6659	CD1	TYR	B	137	1084	1200	931	-20	-28	-89
ATOM	6661	CE1	TYR	B	137	74.172	28.474	52.929	1.00	8.41	
ANISOU	6661	CE1	TYR	B	137	1046	1076	1072	-32	10	87
ATOM	6663	CZ	TYR	B	137	74.671	28.944	54.149	1.00	7.72	
ANISOU	6663	CZ	TYR	B	137	958	897	1076	-37	91	87
ATOM	6664	OH	TYR	B	137	75.410	30.080	54.226	1.00	8.42	
ANISOU	6664	OH	TYR	B	137	896	941	1359	-155	38	-107
ATOM	6666	CE2	TYR	B	137	74.379	28.295	55.304	1.00	5.35	
ANISOU	6666	CE2	TYR	B	137	523	792	718	208	-123	159
ATOM	6668	CD2	TYR	B	137	73.603	27.079	55.236	1.00	9.47	
ANISOU	6668	CD2	TYR	B	137	1184	1225	1189	64	50	-110
ATOM	6670	C	TYR	B	137	73.600	23.560	54.864	1.00	6.91	
ANISOU	6670	C	TYR	B	137	996	881	748	-6	-54	13
ATOM	6671	O	TYR	B	137	73.138	23.215	55.943	1.00	6.59	

ANISOU	6671	O	TYR	B	137
ATOM	6672	N	HIS	B	138
ANISOU	6672	N	HIS	B	138
ATOM	6674	CA	HIS	B	138
ANISOU	6674	CA	HIS	B	138
ATOM	6676	CB	HIS	B	138
ANISOU	6676	CB	HIS	B	138
ATOM	6679	CG	HIS	B	138
ANISOU	6679	CG	HIS	B	138
ATOM	6680	ND1	HIS	B	138
ANISOU	6680	ND1	HIS	B	138
ATOM	6682	CE1	HIS	B	138
ANISOU	6682	CE1	HIS	B	138
ATOM	6684	NE2	HIS	B	138
ANISOU	6684	NE2	HIS	B	138
ATOM	6686	CD2	HIS	B	138
ANISOU	6686	CD2	HIS	B	138
ATOM	6688	C	HIS	B	138
ANISOU	6688	C	HIS	B	138
ATOM	6689	O	HIS	B	138
ANISOU	6689	O	HIS	B	138
ATOM	6690	N	VAL	B	139
ANISOU	6690	N	VAL	B	139
ATOM	6692	CA	VAL	B	139
ANISOU	6692	CA	VAL	B	139
ATOM	6694	CB	VAL	B	139
ANISOU	6694	CB	VAL	B	139
ATOM	6696	CG1	VAL	B	139
ANISOU	6696	CG1	VAL	B	139
ATOM	6700	CG2	VAL	B	139
ANISOU	6700	CG2	VAL	B	139
ATOM	6704	C	VAL	B	139
ANISOU	6704	C	VAL	B	139
ATOM	6705	O	VAL	B	139
ANISOU	6705	O	VAL	B	139
ATOM	6706	N	LEU	B	140
ANISOU	6706	N	LEU	B	140
ATOM	6834	N	VAL	B	148
ANISOU	6834	N	VAL	B	148
ATOM	6836	CA	VAL	B	148
ANISOU	6836	CA	VAL	B	148
ATOM	6838	CB	VAL	B	148
ANISOU	6838	CB	VAL	B	148
ATOM	6840	CG1	VAL	B	148
ANISOU	6840	CG1	VAL	B	148
ATOM	6844	CG2	VAL	B	148
ANISOU	6844	CG2	VAL	B	148
ATOM	6848	C	VAL	B	148
ANISOU	6848	C	VAL	B	148
ATOM	6849	O	VAL	B	148
ANISOU	6849	O	VAL	B	148
ATOM	6850	N	GLU	B	149
ANISOU	6850	N	GLU	B	149
ATOM	6852	CA	GLU	B	149
ANISOU	6852	CA	GLU	B	149
ATOM	6863	C	GLU	B	149
ANISOU	6863	C	GLU	B	149
ATOM	6864	O	GLU	B	149
ANISOU	6864	O	GLU	B	149
ATOM	6865	N	PHE	B	150
ANISOU	6865	N	PHE	B	150

[illegible]

ATOM	6867	CA	PHE	B	150	71.969	11.579	52.168	1.00	7.78		C
ANISOU	6867	CA	PHE	B	150	941	1007	1005	26	-8	-15	C
ATOM	6869	CB	PHE	B	150	72.739	12.540	51.231	1.00	7.97		C
ANISOU	6869	CB	PHE	B	150	1032	1064	933	28	-2	-2	C
ATOM	6872	CG	PHE	B	150	72.173	13.948	51.206	1.00	8.57		C
ANISOU	6872	CG	PHE	B	150	1195	938	1120	45	-41	93	C
ATOM	6873	CD1	PHE	B	150	72.557	14.895	52.134	1.00	12.11		C
ANISOU	6873	CD1	PHE	B	150	1643	1428	1531	22	-203	54	C
ATOM	6875	CE1	PHE	B	150	72.003	16.216	52.140	1.00	10.64		C
ANISOU	6875	CE1	PHE	B	150	1351	1173	1516	-115	-139	-97	C
ATOM	6877	CZ	PHE	B	150	71.046	16.534	51.256	1.00	10.18		C
ANISOU	6877	CZ	PHE	B	150	1334	1242	1290	-130	40	-33	C
ATOM	6879	CE2	PHE	B	150	70.623	15.549	50.351	1.00	11.13		C
ANISOU	6879	CE2	PHE	B	150	1491	1469	1268	38	-131	-124	C
ATOM	6881	CD2	PHE	B	150	71.171	14.282	50.341	1.00	10.74		C
ANISOU	6881	CD2	PHE	B	150	1347	1344	1386	-85	-161	29	C
ATOM	6883	C	PHE	B	150	72.700	10.265	52.100	1.00	8.82		C
ANISOU	6883	C	PHE	B	150	1038	1171	1142	64	-21	63	C
ATOM	6884	O	PHE	B	150	73.608	10.019	52.917	1.00	8.69		O
ANISOU	6884	O	PHE	B	150	998	1272	1031	219	-107	-17	O
ATOM	6885	N	ASP	B	151	72.365	9.462	51.099	1.00	7.95		N
ANISOU	6885	N	ASP	B	151	855	1103	1063	54	-26	-36	N
ATOM	6887	CA	ASP	B	151	73.146	8.247	50.874	1.00	11.66		C
ANISOU	6887	CA	ASP	B	151	1462	1489	1478	-6	46	0	C
ATOM	6893	OD1	ASP	B	151	72.308	8.468	48.189	1.00	14.12		O
ANISOU	6893	OD1	ASP	B	151	2159	1645	1560	-238	-102	-219	O
ATOM	6895	C	ASP	B	151	74.422	8.605	50.100	1.00	12.63		C
ANISOU	6895	C	ASP	B	151	1537	1674	1588	-69	97	-21	C
ATOM	6896	O	ASP	B	151	74.642	9.780	49.779	1.00	12.87		O
ANISOU	6896	O	ASP	B	151	1663	1654	1569	-70	101	-32	O
ATOM	6897	N	GLN	B	152	75.215	7.600	49.759	1.00	14.56		N
ANISOU	6897	N	GLN	B	152	1777	1810	1944	32	9	118	N
ATOM	6899	CA	GLN	B	152	76.488	7.838	49.037	1.00	17.68		C
ANISOU	6899	CA	GLN	B	152	2162	2279	2274	14	76	1	C
ATOM	6912	C	GLN	B	152	76.263	8.376	47.652	1.00	17.50		C
ANISOU	6912	C	GLN	B	152	2171	2225	2250	72	32	10	C
ATOM	6913	O	GLN	B	152	77.173	8.900	47.045	1.00	19.80		O
ANISOU	6913	O	GLN	B	152	2439	2641	2443	139	-13	43	O
ATOM	6914	N	GLY	B	153	75.053	8.272	47.131	1.00	18.53		N
ANISOU	6914	N	GLY	B	153	2378	2348	2312	57	43	-40	N
ATOM	6916	CA	GLY	B	153	74.773	8.831	45.820	1.00	18.90		C
ANISOU	6916	CA	GLY	B	153	2436	2448	2296	84	37	-55	C
ATOM	6919	C	GLY	B	153	74.248	10.248	45.806	1.00	19.41		C
ANISOU	6919	C	GLY	B	153	2552	2497	2323	34	25	20	C
ATOM	6920	O	GLY	B	153	74.055	10.805	44.731	1.00	20.09		O
ANISOU	6920	O	GLY	B	153	2598	2890	2145	145	11	-51	O
ATOM	6921	N	GLY	B	154	74.036	10.850	46.984	1.00	18.63		N
ANISOU	6921	N	GLY	B	154	2469	2370	2237	28	46	-33	N
ATOM	6923	CA	GLY	B	154	73.537	12.212	47.068	1.00	18.75		C
ANISOU	6923	CA	GLY	B	154	2451	2422	2248	-18	-6	-15	C
ATOM	6926	C	GLY	B	154	72.049	12.274	47.245	1.00	18.31		C
ANISOU	6926	C	GLY	B	154	2411	2345	2198	15	10	-8	C
ATOM	6927	O	GLY	B	154	71.453	13.346	47.239	1.00	20.30		O
ANISOU	6927	O	GLY	B	154	2655	2699	2358	82	11	-60	O
ATOM	6928	N	LYS	B	155	71.425	11.117	47.411	1.00	17.75		N
ANISOU	6928	N	LYS	B	155	2314	2317	2110	37	12	-80	N
ATOM	6930	CA	LYS	B	155	69.988	11.059	47.555	1.00	17.17		C
ANISOU	6930	CA	LYS	B	155	2180	2237	2103	91	28	-17	C
ATOM	6932	CB	LYS	B	155	69.482	9.761	47.002	1.00	17.96		C
ANISOU	6932	CB	LYS	B	155	2303	2430	2091	-12	-30	-48	C
ATOM	6935	CG	LYS	B	155	67.966	9.620	47.005	1.00	21.83		C

ANISOU	6935	CG	LYS B	155	2640	2916	2737	15	77	-3	C
ATOM	6948	C	LYS B	155	69.559	11.180	49.042	1.00	15.76		C
ANISOU	6948	C	LYS B	155	2059	2050	1878	124	-21	-73	C
ATOM	6949	O	LYS B	155	70.065	10.465	49.938	1.00	14.36		O
ANISOU	6949	O	LYS B	155	1609	1920	1924	334	-186	-205	O
ATOM	6950	N	ALA B	156	68.603	12.075	49.285	1.00	13.95		N
ANISOU	6950	N	ALA B	156	1638	1987	1674	152	-62	-70	N
ATOM	6952	CA	ALA B	156	68.012	12.259	50.637	1.00	13.87		C
ANISOU	6952	CA	ALA B	156	1728	1857	1685	94	-29	-28	C
ATOM	6954	CB	ALA B	156	66.884	13.323	50.575	1.00	13.88		C
ANISOU	6954	CB	ALA B	156	1673	1783	1815	19	-75	-91	C
ATOM	6958	C	ALA B	156	67.393	10.975	51.100	1.00	13.28		C
ANISOU	6958	C	ALA B	156	1610	1744	1690	112	-29	-165	C
ATOM	7147	CA	SER B	168	74.913	15.048	58.788	1.00	8.49		C
ANISOU	7147	CA	SER B	168	964	1151	1110	2	-31	-32	C
ATOM	7149	CB	SER B	168	74.321	15.086	57.392	1.00	7.62		C
ANISOU	7149	CB	SER B	168	888	1013	992	-25	-44	-109	C
ATOM	7152	OG	SER B	168	73.281	16.077	57.307	1.00	8.98		O
ANISOU	7152	OG	SER B	168	826	1444	1140	53	-406	-271	O
ATOM	7154	C	SER B	168	75.000	16.498	59.258	1.00	8.20		C
ANISOU	7154	C	SER B	168	925	1116	1075	27	-72	-66	C
ATOM	7156	N	ASN B	169	75.720	17.311	58.516	1.00	8.34		N
ANISOU	7156	N	ASN B	169	1082	1134	953	33	-28	12	N
ATOM	7158	CA	ASN B	169	75.830	18.723	58.792	1.00	9.44		C
ANISOU	7158	CA	ASN B	169	1280	1219	1087	60	21	-29	C
ATOM	7160	CB	ASN B	169	77.288	19.190	58.675	1.00	10.02		C
ANISOU	7160	CB	ASN B	169	1439	1222	1145	1	-50	-65	C
ATOM	7163	CG	ASN B	169	78.135	18.686	59.862	1.00	11.94		C
ANISOU	7163	CG	ASN B	169	1572	1549	1415	80	-166	-103	C
ATOM	7165	ND2	ASN B	169	79.280	18.144	59.581	1.00	10.28		N
ANISOU	7165	ND2	ASN B	169	1387	1439	1079	3	-271	-63	N
ATOM	7168	C	ASN B	169	74.902	19.558	57.911	1.00	9.68		C
ANISOU	7168	C	ASN B	169	1384	1215	1077	-22	-80	-15	C
ATOM	7169	O	ASN B	169	75.076	20.779	57.793	1.00	10.98		O
ANISOU	7169	O	ASN B	169	1808	1180	1180	-171	-94	-73	O
ATOM	7170	N	TYR B	170	73.947	18.924	57.249	1.00	8.76		N
ANISOU	7170	N	TYR B	170	1193	1035	1100	-16	82	-62	N
ATOM	7172	CA	TYR B	170	73.041	19.648	56.357	1.00	6.97		C
ANISOU	7172	CA	TYR B	170	859	947	839	-65	20	-13	C
ATOM	7174	CB	TYR B	170	72.838	18.873	55.047	1.00	7.14		C
ANISOU	7174	CB	TYR B	170	744	1100	869	27	64	-56	C
ATOM	7177	CG	TYR B	170	74.049	19.087	54.169	1.00	6.20		C
ANISOU	7177	CG	TYR B	170	682	865	806	-82	28	84	C
ATOM	7178	CD1	TYR B	170	75.125	18.210	54.227	1.00	7.09		C
ANISOU	7178	CD1	TYR B	170	881	1015	797	-42	-24	-21	C
ATOM	7180	CE1	TYR B	170	76.267	18.445	53.502	1.00	6.23		C
ANISOU	7180	CE1	TYR B	170	789	825	751	-21	92	-81	C
ATOM	7182	CZ	TYR B	170	76.319	19.611	52.703	1.00	8.76		C
ANISOU	7182	CZ	TYR B	170	1264	1229	833	-31	-143	-45	C
ATOM	7183	OH	TYR B	170	77.437	19.928	51.984	1.00	10.49		O
ANISOU	7183	OH	TYR B	170	1549	1362	1073	-217	90	-84	O
ATOM	7185	CE2	TYR B	170	75.288	20.489	52.678	1.00	8.94		C
ANISOU	7185	CE2	TYR B	170	1111	1124	1159	-72	148	-78	C
ATOM	7187	CD2	TYR B	170	74.161	20.230	53.421	1.00	7.63		C
ANISOU	7187	CD2	TYR B	170	1007	924	965	-99	42	-17	C
ATOM	7189	C	TYR B	170	71.705	19.966	56.998	1.00	8.15		C
ANISOU	7189	C	TYR B	170	980	1052	1062	-14	4	-7	C
ATOM	7190	O	TYR B	170	70.939	19.041	57.332	1.00	9.22		O
ANISOU	7190	O	TYR B	170	1159	1096	1248	-254	192	159	O
ATOM	7191	N	ALA B	171	71.437	21.251	57.213	1.00	7.85		N
ANISOU	7191	N	ALA B	171	922	915	1145	-85	-3	128	N

ATOM	7193	CA	ALA B 171	70.157	21.703	57.779	1.00	6.04		C
ANISOU	7193	CA	ALA B 171	830	722	741	-16	-7	129	C
ATOM	7195	CB	ALA B 171	70.345	23.032	58.562	1.00	7.20		C
ANISOU	7195	CB	ALA B 171	910	977	845	34	-101	113	C
ATOM	7199	C	ALA B 171	69.182	21.939	56.641	1.00	7.69		C
ANISOU	7199	C	ALA B 171	914	1065	940	-10	-11	60	C
ATOM	7200	O	ALA B 171	69.585	22.371	55.569	1.00	9.49		O
ANISOU	7200	O	ALA B 171	1245	1401	958	41	-59	75	O
ATOM	7201	N	VAL B 172	67.904	21.754	56.929	1.00	7.02		N
ANISOU	7201	N	VAL B 172	877	941	849	-86	37	83	N
ATOM	7203	CA	VAL B 172	66.820	22.038	55.994	1.00	7.98		C
ANISOU	7203	CA	VAL B 172	986	1067	978	-7	60	93	C
ATOM	7205	CB	VAL B 172	65.689	21.006	56.048	1.00	7.69		C
ANISOU	7205	CB	VAL B 172	860	985	1074	13	10	81	C
ATOM	7207	CG1	VAL B 172	64.547	21.391	55.088	1.00	7.84		C
ANISOU	7207	CG1	VAL B 172	1162	1028	787	-190	-64	125	C
ATOM	7211	CG2	VAL B 172	66.192	19.558	55.778	1.00	8.46		C
ANISOU	7211	CG2	VAL B 172	1103	1224	887	-156	204	-81	C
ATOM	7215	C	VAL B 172	66.365	23.443	56.381	1.00	8.06		C
ANISOU	7215	C	VAL B 172	967	1038	1058	-44	8	38	C
ATOM	7217	N	THR B 173	66.585	24.394	55.469	1.00	9.20		N
ANISOU	7217	N	THR B 173	1211	1258	1024	32	28	12	N
ATOM	7219	CA	THR B 173	66.371	25.812	55.744	1.00	9.64		C
ANISOU	7219	CA	THR B 173	1185	1226	1249	26	17	75	C
ATOM	7221	CB	THR B 173	67.023	26.735	54.707	1.00	9.14		C
ANISOU	7221	CB	THR B 173	1041	1285	1147	96	122	-4	C
ATOM	7223	OG1	THR B 173	66.266	26.732	53.499	1.00	10.36		O
ANISOU	7223	OG1	THR B 173	1012	1431	1493	-10	304	28	O
ATOM	7225	CG2	THR B 173	68.470	26.306	54.352	1.00	10.18		C
ANISOU	7225	CG2	THR B 173	1304	1372	1190	-76	229	162	C
ATOM	7251	CD2	LEU B 175	63.498	29.481	49.870	1.00	12.70		C
ANISOU	7251	CD2	LEU B 175	1717	1586	1521	-282	120	-139	C
ATOM	7865	N	SER B 213	61.913	16.976	46.696	1.00	7.08		N
ANISOU	7865	N	SER B 213	674	925	1090	-11	-47	-55	N
ATOM	7867	CA	SER B 213	63.154	17.422	46.071	1.00	6.55		C
ANISOU	7867	CA	SER B 213	793	829	866	-92	66	4	C
ATOM	7869	CB	SER B 213	62.831	18.416	45.000	1.00	6.60		C
ANISOU	7869	CB	SER B 213	545	1032	927	11	-196	18	C
ATOM	7872	OG	SER B 213	64.004	18.999	44.434	1.00	9.48		O
ANISOU	7872	OG	SER B 213	1094	1226	1281	-117	432	256	O
ATOM	7874	C	SER B 213	63.971	18.198	47.116	1.00	7.04		C
ANISOU	7874	C	SER B 213	877	1011	787	23	-55	-22	C
ATOM	7875	O	SER B 213	63.527	19.266	47.564	1.00	8.08		O
ANISOU	7875	O	SER B 213	1033	1179	858	-38	4	-193	O
ATOM	7876	N	VAL B 214	65.176	17.725	47.420	1.00	7.32		N
ANISOU	7876	N	VAL B 214	907	960	914	-22	27	-86	N
ATOM	7878	CA	VAL B 214	66.065	18.412	48.332	1.00	8.50		C
ANISOU	7878	CA	VAL B 214	992	1117	1118	26	-31	7	C
ATOM	7880	CB	VAL B 214	66.662	17.473	49.325	1.00	9.49		C
ANISOU	7880	CB	VAL B 214	1135	1234	1236	-41	-99	20	C
ATOM	7882	CG1	VAL B 214	67.640	18.265	50.220	1.00	9.17		C
ANISOU	7882	CG1	VAL B 214	1216	1187	1081	158	-197	-2	C
ATOM	7886	CG2	VAL B 214	65.557	16.808	50.137	1.00	11.30		C
ANISOU	7886	CG2	VAL B 214	1389	1327	1576	58	-56	153	C
ATOM	7890	C	VAL B 214	67.181	18.986	47.493	1.00	8.26		C
ANISOU	7890	C	VAL B 214	916	1055	1164	-59	-44	-4	C
ATOM	7891	O	VAL B 214	67.989	18.241	46.905	1.00	9.17		O
ANISOU	7891	O	VAL B 214	800	1215	1469	-74	237	171	O
ATOM	7892	N	GLU B 215	67.172	20.293	47.357	1.00	8.23		N
ANISOU	7892	N	GLU B 215	917	1057	1150	26	-148	-24	N
ATOM	7894	CA	GLU B 215	68.211	20.975	46.602	1.00	9.54		C

ANISOU	7894	CA	GLU	B	215	1134	1246	1244	5	1	10	C
ATOM	7896	CB	GLU	B	215	67.662	22.184	45.830	1.00	10.10		C
ANISOU	7896	CB	GLU	B	215	1238	1336	1261	-114	-15	54	C
ATOM	7899	CG	GLU	B	215	66.611	21.801	44.781	1.00	13.81		C
ANISOU	7899	CG	GLU	B	215	1578	1910	1758	-121	-99	21	C
ATOM	7902	CD	GLU	B	215	67.090	21.091	43.527	1.00	17.31		C
ANISOU	7902	CD	GLU	B	215	2165	2407	2002	-22	15	-95	C
ATOM	7903	OE1	GLU	B	215	68.286	21.016	43.241	1.00	18.35		O
ANISOU	7903	OE1	GLU	B	215	2158	2601	2211	-189	-201	-105	O
ATOM	7904	OE2	GLU	B	215	66.196	20.584	42.790	1.00	18.32		O
ANISOU	7904	OE2	GLU	B	215	2329	2396	2235	-24	-109	123	O
ATOM	7905	C	GLU	B	215	69.311	21.454	47.534	1.00	10.31		C
ANISOU	7905	C	GLU	B	215	1285	1363	1268	-32	-7	35	C
ATOM	7906	O	GLU	B	215	69.015	21.990	48.613	1.00	10.95		O
ANISOU	7906	O	GLU	B	215	1164	1485	1511	-3	42	-262	O
ATOM	7907	N	ILE	B	216	70.582	21.269	47.143	1.00	8.84		N
ANISOU	7907	N	ILE	B	216	1186	1120	1050	17	136	-41	N
ATOM	7909	CA	ILE	B	216	71.663	21.828	47.943	1.00	9.55		C
ANISOU	7909	CA	ILE	B	216	1186	1120	1323	-38	53	154	C
ATOM	7911	CB	ILE	B	216	73.019	21.179	47.676	1.00	9.77		C
ANISOU	7911	CB	ILE	B	216	1333	987	1390	-102	84	95	C
ATOM	7913	CG1	ILE	B	216	72.965	19.655	47.786	1.00	10.93		C
ANISOU	7913	CG1	ILE	B	216	1542	1161	1448	140	-36	77	C
ATOM	7916	CD1	ILE	B	216	72.520	19.201	49.103	1.00	12.05		C
ANISOU	7916	CD1	ILE	B	216	1598	1323	1658	92	147	24	C
ATOM	7920	CG2	ILE	B	216	74.070	21.754	48.722	1.00	13.23		C
ANISOU	7920	CG2	ILE	B	216	1725	1640	1660	77	-40	68	C
ATOM	7924	C	ILE	B	216	71.764	23.376	47.628	1.00	9.10		C
ANISOU	7924	C	ILE	B	216	1022	1150	1284	-74	58	42	C
ATOM	7925	O	ILE	B	216	71.927	23.788	46.438	1.00	8.37		O
ANISOU	7925	O	ILE	B	216	843	1177	1158	-225	-132	135	O
ATOM	7926	N	MET	B	217	71.750	24.157	48.702	1.00	7.68		N
ANISOU	7926	N	MET	B	217	609	1083	1225	-68	47	-9	N
ATOM	7928	CA	MET	B	217	72.067	25.557	48.649	1.00	8.58		C
ANISOU	7928	CA	MET	B	217	947	1130	1180	11	-66	39	C
ATOM	7930	CB	MET	B	217	71.215	26.316	49.614	1.00	9.01		C
ANISOU	7930	CB	MET	B	217	1087	1149	1187	-42	-41	-31	C
ATOM	7933	CG	MET	B	217	71.532	27.850	49.786	1.00	10.49		C
ANISOU	7933	CG	MET	B	217	1444	1082	1457	-75	-43	172	C
ATOM	7936	SD	MET	B	217	70.285	28.672	50.856	1.00	12.06		S
ANISOU	7936	SD	MET	B	217	1553	1472	1554	196	-5	-92	S
ATOM	7937	CE	MET	B	217	68.809	28.514	49.872	1.00	13.78		C
ANISOU	7937	CE	MET	B	217	1799	1689	1747	-59	188	138	C
ATOM	7941	C	MET	B	217	73.554	25.671	49.012	1.00	7.98		C
ANISOU	7941	C	MET	B	217	960	984	1088	-4	-22	-25	C
ATOM	7942	O	MET	B	217	73.983	25.471	50.156	1.00	9.87		O
ANISOU	7942	O	MET	B	217	1136	1378	1233	46	-49	97	O
ATOM	7943	N	GLY	B	218	74.336	26.021	48.037	1.00	6.93		N
ANISOU	7943	N	GLY	B	218	706	873	1053	42	0	-36	N
ATOM	7945	CA	GLY	B	218	75.763	25.985	48.251	1.00	7.75		C
ANISOU	7945	CA	GLY	B	218	864	1131	947	-81	-97	87	C
ATOM	7948	C	GLY	B	218	76.297	27.058	49.196	1.00	6.37		C
ANISOU	7948	C	GLY	B	218	761	859	800	-65	36	0	C
ATOM	7949	O	GLY	B	218	75.642	28.068	49.536	1.00	7.36		O
ANISOU	7949	O	GLY	B	218	587	1263	945	-128	-52	-133	O
ATOM	7950	N	ARG	B	219	77.558	26.840	49.549	1.00	6.20		N
ANISOU	7950	N	ARG	B	219	806	840	710	72	-118	12	N
ATOM	7952	CA	ARG	B	219	78.279	27.638	50.533	1.00	7.04		C
ANISOU	7952	CA	ARG	B	219	886	882	907	-45	22	-10	C
ATOM	7954	CB	ARG	B	219	79.628	26.957	50.844	1.00	7.14		C
ANISOU	7954	CB	ARG	B	219	952	863	896	36	-60	-26	C

ATOM	7957	CG	ARG B 219	80.628	26.960	49.706	1.00	8.87		C
ANISOU	7957	CG	ARG B 219	1149	1134	1086	-17	-70	26	C
ATOM	7960	CD	ARG B 219	81.710	25.866	49.818	1.00	7.79		C
ANISOU	7960	CD	ARG B 219	949	1126	882	-107	134	61	C
ATOM	7963	NE	ARG B 219	82.748	26.206	50.807	1.00	9.90		N
ANISOU	7963	NE	ARG B 219	1196	1491	1074	14	-52	47	N
ATOM	7965	CZ	ARG B 219	83.739	25.379	51.123	1.00	10.34		C
ANISOU	7965	CZ	ARG B 219	1423	1320	1182	-15	-102	72	C
ATOM	7966	NH1	ARG B 219	83.743	24.157	50.604	1.00	11.14		N
ANISOU	7966	NH1	ARG B 219	1526	1458	1247	103	102	-40	N
ATOM	7969	NH2	ARG B 219	84.683	25.734	52.002	1.00	7.84		N
ANISOU	7969	NH2	ARG B 219	996	873	1108	23	-20	124	N
ATOM	7972	C	ARG B 219	78.484	29.081	50.080	1.00	7.31		C
ANISOU	7972	C	ARG B 219	964	858	955	99	-33	-59	C
ATOM	7973	O	ARG B 219	78.874	29.954	50.862	1.00	7.45		O
ANISOU	7973	O	ARG B 219	779	964	1087	54	10	-205	O
ATOM	7974	N	GLY B 220	78.387	29.287	48.780	1.00	6.52		N
ANISOU	7974	N	GLY B 220	907	787	781	-8	25	42	N
ATOM	7976	CA	GLY B 220	78.409	30.629	48.260	1.00	8.26		C
ANISOU	7976	CA	GLY B 220	1232	1001	905	81	-41	-29	C
ATOM	7979	C	GLY B 220	77.242	31.516	48.666	1.00	7.37		C
ANISOU	7979	C	GLY B 220	929	1039	830	70	-106	3	C
ATOM	7980	O	GLY B 220	77.418	32.743	48.606	1.00	8.65		O
ANISOU	7980	O	GLY B 220	1099	1119	1068	340	-111	55	O
ATOM	7981	N	TYR B 221	76.114	30.929	49.092	1.00	7.64		N
ANISOU	7981	N	TYR B 221	1072	1041	787	37	-28	-12	N
ATOM	7983	CA	TYR B 221	74.967	31.663	49.586	1.00	7.64		C
ANISOU	7983	CA	TYR B 221	1014	1017	870	92	-155	90	C
ATOM	7985	CB	TYR B 221	73.672	30.854	49.426	1.00	7.23		C
ANISOU	7985	CB	TYR B 221	960	899	887	60	-74	86	C
ATOM	7988	CG	TYR B 221	73.155	30.704	47.991	1.00	7.13		C
ANISOU	7988	CG	TYR B 221	665	1180	863	-113	31	80	C
ATOM	7989	CD1	TYR B 221	73.196	29.500	47.340	1.00	8.62		C
ANISOU	7989	CD1	TYR B 221	1032	1177	1063	-86	88	261	C
ATOM	7991	CE1	TYR B 221	72.751	29.378	46.037	1.00	10.83		C
ANISOU	7991	CE1	TYR B 221	1308	1493	1311	-316	-130	55	C
ATOM	7993	CZ	TYR B 221	72.198	30.503	45.393	1.00	12.21		C
ANISOU	7993	CZ	TYR B 221	1491	1724	1423	79	-47	-42	C
ATOM	7994	OH	TYR B 221	71.696	30.425	44.065	1.00	14.19		O
ANISOU	7994	OH	TYR B 221	1301	2531	1557	51	-207	160	O
ATOM	7996	CE2	TYR B 221	72.128	31.685	46.046	1.00	10.38		C
ANISOU	7996	CE2	TYR B 221	1243	1385	1313	-184	-82	331	C
ATOM	7998	CD2	TYR B 221	72.588	31.791	47.329	1.00	9.62		C
ANISOU	7998	CD2	TYR B 221	1246	1172	1235	-163	63	-24	C
ATOM	8000	C	TYR B 221	75.110	31.869	51.094	1.00	8.55		C
ANISOU	8000	C	TYR B 221	1222	1053	971	35	-17	-38	C
ATOM	8001	O	TYR B 221	75.737	31.045	51.754	1.00	9.15		O
ANISOU	8001	O	TYR B 221	1659	1026	790	301	-188	-143	O
ATOM	8002	N	ALA B 222	74.590	32.977	51.612	1.00	8.75		N
ANISOU	8002	N	ALA B 222	1042	1052	1230	134	29	102	N
ATOM	8004	CA	ALA B 222	74.490	33.151	53.032	1.00	9.59		C
ANISOU	8004	CA	ALA B 222	1092	1207	1344	87	-1	51	C
ATOM	8006	CB	ALA B 222	74.801	34.548	53.454	1.00	11.40		C
ANISOU	8006	CB	ALA B 222	1295	1475	1559	-94	103	-38	C
ATOM	8010	C	ALA B 222	73.055	32.801	53.417	1.00	10.24		C
ANISOU	8010	C	ALA B 222	1158	1337	1395	-75	98	121	C
ATOM	8011	O	ALA B 222	72.111	33.257	52.772	1.00	8.71		O
ANISOU	8011	O	ALA B 222	748	1108	1453	-277	191	100	O
ATOM	8012	N	TRP B 223	72.927	31.966	54.433	1.00	10.57		N
ANISOU	8012	N	TRP B 223	1245	1424	1345	17	81	91	N
ATOM	8014	CA	TRP B 223	71.617	31.648	55.060	1.00	9.73		C

ANISOU	8014	CA	TRP	B	223	1096	1348	1250	-25	-9	12	C
ATOM	8016	CB	TRP	B	223	71.184	30.192	54.891	1.00	10.75		C
ANISOU	8016	CB	TRP	B	223	1287	1554	1243	-72	26	34	C
ATOM	8019	CG	TRP	B	223	69.899	29.871	55.706	1.00	8.42		C
ANISOU	8019	CG	TRP	B	223	965	1209	1024	-108	-24	-124	C
ATOM	8020	CD1	TRP	B	223	68.777	30.564	55.722	1.00	11.01		C
ANISOU	8020	CD1	TRP	B	223	1576	1392	1216	-25	-62	78	C
ATOM	8022	NE1	TRP	B	223	67.868	30.014	56.604	1.00	10.77		N
ANISOU	8022	NE1	TRP	B	223	1066	1479	1544	-85	238	46	N
ATOM	8024	CE2	TRP	B	223	68.482	28.978	57.262	1.00	9.41		C
ANISOU	8024	CE2	TRP	B	223	1173	1284	1116	88	205	-33	C
ATOM	8025	CD2	TRP	B	223	69.753	28.847	56.705	1.00	10.61		C
ANISOU	8025	CD2	TRP	B	223	1055	1431	1545	-103	35	2	C
ATOM	8026	CE3	TRP	B	223	70.584	27.825	57.182	1.00	10.23		C
ANISOU	8026	CE3	TRP	B	223	1311	1107	1466	-59	-10	144	C
ATOM	8028	CZ3	TRP	B	223	70.117	26.979	58.160	1.00	9.84		C
ANISOU	8028	CZ3	TRP	B	223	1148	1407	1182	45	95	-61	C
ATOM	8034	C	TRP	B	223	71.869	31.908	56.530	1.00	12.21		C
ANISOU	8034	C	TRP	B	223	1507	1706	1426	23	106	131	C
ATOM	8035	O	TRP	B	223	72.679	31.207	57.206	1.00	12.56		O
ANISOU	8035	O	TRP	B	223	1512	1769	1490	191	130	164	O
ATOM	8036	N	LEU	B	224	71.202	32.910	57.044	1.00	13.37		N
ANISOU	8036	N	LEU	B	224	1845	1630	1605	125	-8	85	N
ATOM	8038	CA	LEU	B	224	71.365	33.268	58.431	1.00	16.15		C
ANISOU	8038	CA	LEU	B	224	2148	1939	2046	20	-24	-15	C
ATOM	8043	CG	LEU	B	224	73.181	34.812	57.629	1.00	16.95		C
ANISOU	8043	CG	LEU	B	224	2208	2006	2223	-30	-11	-31	C
ATOM	8045	CD1	LEU	B	224	73.511	36.294	57.545	1.00	17.91		C
ANISOU	8045	CD1	LEU	B	224	2639	2042	2123	-104	95	-78	C
ATOM	8049	CD2	LEU	B	224	74.332	33.994	58.192	1.00	16.82		C
ANISOU	8049	CD2	LEU	B	224	2057	2028	2304	-97	-33	-44	C
ATOM	8237	CG	PHE	B	238	76.258	39.198	55.928	1.00	11.60		C
ANISOU	8237	CG	PHE	B	238	1602	1349	1453	-201	86	1	C
ATOM	8238	CD1	PHE	B	238	77.325	38.359	55.898	1.00	14.20		C
ANISOU	8238	CD1	PHE	B	238	1878	1593	1923	-184	230	-20	C
ATOM	8240	CE1	PHE	B	238	77.563	37.545	54.819	1.00	17.85		C
ANISOU	8240	CE1	PHE	B	238	2698	2083	2001	-70	-2	-56	C
ATOM	8242	CZ	PHE	B	238	76.710	37.550	53.782	1.00	16.16		C
ANISOU	8242	CZ	PHE	B	238	2221	1879	2037	-76	-146	-94	C
ATOM	8244	CE2	PHE	B	238	75.662	38.347	53.774	1.00	14.44		C
ANISOU	8244	CE2	PHE	B	238	1901	1679	1905	-159	402	-28	C
ATOM	8246	CD2	PHE	B	238	75.406	39.189	54.909	1.00	15.83		C
ANISOU	8246	CD2	PHE	B	238	2434	1791	1786	-218	-94	11	C
ATOM	8287	CG2	THR	B	241	80.981	44.091	54.329	1.00	10.17		C
ANISOU	8287	CG2	THR	B	241	1011	1501	1352	101	-35	70	C
ATOM	8295	CA	LEU	B	242	77.280	44.645	51.519	1.00	9.28		C
ANISOU	8295	CA	LEU	B	242	1236	1175	1112	60	39	-11	C
ATOM	8297	CB	LEU	B	242	76.281	43.555	51.232	1.00	7.76		C
ANISOU	8297	CB	LEU	B	242	916	1129	902	-10	71	213	C
ATOM	8300	CG	LEU	B	242	76.869	42.164	51.479	1.00	12.76		C
ANISOU	8300	CG	LEU	B	242	1718	1540	1588	50	111	29	C
ATOM	8302	CD1	LEU	B	242	75.784	41.132	51.539	1.00	14.27		C
ANISOU	8302	CD1	LEU	B	242	1867	1780	1772	-47	10	-24	C
ATOM	8306	CD2	LEU	B	242	77.885	41.781	50.462	1.00	13.59		C
ANISOU	8306	CD2	LEU	B	242	1684	1512	1967	82	128	-47	C
ATOM	8348	CG	ARG	B	245	81.698	46.720	48.611	1.00	6.78		C
ANISOU	8348	CG	ARG	B	245	927	895	752	234	-169	38	C
ATOM	8354	NE	ARG	B	245	83.975	46.857	47.851	1.00	7.02		N
ANISOU	8354	NE	ARG	B	245	1161	656	848	260	-263	-45	N
ATOM	8360	NH2	ARG	B	245	85.939	46.653	46.748	1.00	12.77		N
ANISOU	8360	NH2	ARG	B	245	1821	1633	1397	-12	97	40	N

ATOM	8372	CG	GLN	B	246	77.461	45.847	46.729	1.00	6.40		C
ANISOU	8372	CG	GLN	B	246	868	968	595	185	166	160	C
ATOM	8375	CD	GLN	B	246	76.489	44.724	46.642	1.00	8.67		C
ANISOU	8375	CD	GLN	B	246	1178	1137	976	146	4	182	C
ATOM	8377	NE2	GLN	B	246	77.025	43.476	46.649	1.00	9.11		N
ANISOU	8377	NE2	GLN	B	246	1491	991	979	135	86	-126	N
ATOM	9400	CB	PRO	C	17	97.800	29.455	58.563	1.00	34.98		C
ANISOU	9400	CB	PRO	C	17	4463	4437	4388	12	-22	14	C
ATOM	9403	CG	PRO	C	17	96.330	28.941	58.580	1.00	35.79		C
ANISOU	9403	CG	PRO	C	17	4519	4590	4487	-9	-19	-6	C
ATOM	9406	CD	PRO	C	17	95.684	29.442	59.846	1.00	36.57		C
ANISOU	9406	CD	PRO	C	17	4638	4662	4594	-27	-8	3	C
ATOM	13815	CD1	ILE	D	6	98.652	34.855	44.755	1.00	11.24		C
ANISOU	13815	CD1	ILE	D	6	967	1715	1587	-99	147	55	C
ATOM	14147	C	PRO	D	28	93.756	38.921	58.263	1.00	18.28		C
ANISOU	14147	C	PRO	D	28	2471	2236	2236	-11	0	-41	C
ATOM	14149	N	VAL	D	29	92.958	38.211	57.453	1.00	15.26		N
ANISOU	14149	N	VAL	D	29	1989	1914	1894	81	-47	-39	N
ATOM	14151	CA	VAL	D	29	91.550	38.532	57.299	1.00	14.49		C
ANISOU	14151	CA	VAL	D	29	1971	1829	1704	8	-22	-42	C
ATOM	14153	CB	VAL	D	29	91.037	38.537	55.861	1.00	13.03		C
ANISOU	14153	CB	VAL	D	29	1637	1655	1657	-27	-148	-15	C
ATOM	14155	CG1	VAL	D	29	89.523	38.782	55.855	1.00	15.29		C
ANISOU	14155	CG1	VAL	D	29	2005	1845	1958	44	49	47	C
ATOM	14159	CG2	VAL	D	29	91.722	39.594	55.059	1.00	11.37		C
ANISOU	14159	CG2	VAL	D	29	1427	1560	1333	169	-206	-91	C
ATOM	14163	C	VAL	D	29	90.873	37.481	58.152	1.00	13.14		C
ANISOU	14163	C	VAL	D	29	1697	1686	1608	8	-31	-12	C
ATOM	14164	O	VAL	D	29	90.679	36.338	57.744	1.00	13.08		O
ANISOU	14164	O	VAL	D	29	1822	1770	1377	126	-128	160	O
ATOM	14165	N	TYR	D	30	90.528	37.878	59.366	1.00	12.71		N
ANISOU	14165	N	TYR	D	30	1717	1629	1483	-42	-30	45	N
ATOM	14167	CA	TYR	D	30	89.917	36.961	60.338	1.00	13.61		C
ANISOU	14167	CA	TYR	D	30	1794	1757	1620	-68	4	1	C
ATOM	14169	CB	TYR	D	30	88.625	36.297	59.903	1.00	12.88		C
ANISOU	14169	CB	TYR	D	30	1773	1774	1344	2	26	0	C
ATOM	14172	CG	TYR	D	30	87.996	35.415	60.974	1.00	12.15		C
ANISOU	14172	CG	TYR	D	30	1410	1641	1562	-33	-45	-48	C
ATOM	14173	CD1	TYR	D	30	87.839	35.893	62.283	1.00	12.33		C
ANISOU	14173	CD1	TYR	D	30	1424	1787	1471	79	-16	-8	C
ATOM	14175	CE1	TYR	D	30	87.224	35.133	63.263	1.00	11.25		C
ANISOU	14175	CE1	TYR	D	30	1378	1648	1248	-103	-270	180	C
ATOM	14177	CZ	TYR	D	30	86.842	33.817	62.970	1.00	11.44		C
ANISOU	14177	CZ	TYR	D	30	1314	1558	1474	63	-186	-25	C
ATOM	14178	OH	TYR	D	30	86.227	32.988	63.919	1.00	15.52		O
ANISOU	14178	OH	TYR	D	30	1962	2030	1906	98	-314	130	O
ATOM	14180	CE2	TYR	D	30	87.024	33.334	61.713	1.00	10.95		C
ANISOU	14180	CE2	TYR	D	30	1467	1195	1496	-41	-88	-51	C
ATOM	14182	CD2	TYR	D	30	87.633	34.108	60.729	1.00	10.27		C
ANISOU	14182	CD2	TYR	D	30	1319	1564	1018	18	-61	-85	C
ATOM	14184	C	TYR	D	30	90.868	35.901	60.811	1.00	14.13		C
ANISOU	14184	C	TYR	D	30	1912	1734	1723	-96	-28	40	C
ATOM	14185	O	TYR	D	30	91.460	36.112	61.832	1.00	16.09		O
ANISOU	14185	O	TYR	D	30	2347	1950	1817	-183	-19	-48	O
ATOM	14186	N	ASP	D	31	91.051	34.790	60.096	1.00	13.59		N
ANISOU	14186	N	ASP	D	31	1877	1833	1451	-38	36	-64	N
ATOM	14188	CA	ASP	D	31	91.725	33.605	60.642	1.00	13.48		C
ANISOU	14188	CA	ASP	D	31	1683	1815	1622	-90	-7	-27	C
ATOM	14190	CB	ASP	D	31	90.711	32.435	60.909	1.00	14.66		C
ANISOU	14190	CB	ASP	D	31	1849	1985	1735	-136	-28	-99	C
ATOM	14193	CG	ASP	D	31	89.882	32.053	59.695	1.00	14.55		C

ANISOU14193	CG	ASP	D	31	1815	1942	1769	-25	-22	10	C
ATOM 14194	OD1	ASP	D	31	89.991	32.720	58.652	1.00	13.21		O
ANISOU14194	OD1	ASP	D	31	1607	1940	1471	55	93	-73	O
ATOM 14195	OD2	ASP	D	31	89.066	31.070	59.737	1.00	16.83		O
ANISOU14195	OD2	ASP	D	31	2285	2146	1961	-184	-45	-108	O
ATOM 14196	C	ASP	D	31	92.871	33.073	59.782	1.00	13.68		C
ANISOU14196	C	ASP	D	31	1751	1737	1709	-12	-51	-63	C
ATOM 14197	O	ASP	D	31	93.443	32.051	60.076	1.00	15.61		O
ANISOU14197	O	ASP	D	31	1805	2084	2042	137	-154	41	O
ATOM 14198	N	LYS	D	32	93.162	33.759	58.696	1.00	13.03		N
ANISOU14198	N	LYS	D	32	1644	1753	1550	30	56	1	N
ATOM 14200	CA	LYS	D	32	94.235	33.367	57.758	1.00	11.84		C
ANISOU14200	CA	LYS	D	32	1344	1647	1506	12	-2	-4	C
ATOM 14202	CB	LYS	D	32	93.787	32.322	56.750	1.00	11.86		C
ANISOU14202	CB	LYS	D	32	1374	1623	1507	-11	196	24	C
ATOM 14205	CG	LYS	D	32	92.673	32.731	55.856	1.00	12.00		C
ANISOU14205	CG	LYS	D	32	1603	1565	1390	-64	-79	-16	C
ATOM 14208	CD	LYS	D	32	91.951	31.532	55.143	1.00	9.83		C
ANISOU14208	CD	LYS	D	32	908	1273	1552	252	42	41	C
ATOM 14211	CE	LYS	D	32	90.911	30.958	55.993	1.00	10.88		C
ANISOU14211	CE	LYS	D	32	1342	1343	1446	86	40	88	C
ATOM 14214	NZ	LYS	D	32	89.731	31.898	56.048	1.00	10.04		N
ANISOU14214	NZ	LYS	D	32	1383	796	1636	234	131	-253	N
ATOM 14218	C	LYS	D	32	94.824	34.589	57.052	1.00	11.29		C
ANISOU14218	C	LYS	D	32	1368	1572	1349	73	2	17	C
ATOM 14219	O	LYS	D	32	94.199	35.626	56.881	1.00	9.87		O
ANISOU14219	O	LYS	D	32	1278	1400	1070	96	128	-52	O
ATOM 14220	N	PRO	D	33	96.059	34.444	56.580	1.00	11.10		N
ANISOU14220	N	PRO	D	33	1270	1532	1413	36	48	101	N
ATOM 14221	CA	PRO	D	33	96.752	35.556	55.934	1.00	11.36		C
ANISOU14221	CA	PRO	D	33	1426	1388	1499	24	29	41	C
ATOM 14223	CB	PRO	D	33	98.045	34.932	55.445	1.00	11.62		C
ANISOU14223	CB	PRO	D	33	1358	1490	1566	0	-33	84	C
ATOM 14226	CG	PRO	D	33	98.211	33.647	56.306	1.00	12.82		C
ANISOU14226	CG	PRO	D	33	1335	1648	1887	82	191	237	C
ATOM 14229	CD	PRO	D	33	96.807	33.186	56.534	1.00	12.41		C
ANISOU14229	CD	PRO	D	33	1475	1627	1613	-31	135	88	C
ATOM 14232	C	PRO	D	33	95.963	36.049	54.725	1.00	10.95		C
ANISOU14232	C	PRO	D	33	1312	1372	1474	47	-36	75	C
ATOM 14233	O	PRO	D	33	95.418	35.216	53.964	1.00	11.32		O
ANISOU14233	O	PRO	D	33	1701	1121	1476	36	43	138	O
ATOM 14234	N	MET	D	34	95.992	37.360	54.493	1.00	11.68		N
ANISOU14234	N	MET	D	34	1444	1423	1572	-51	-34	43	N
ATOM 14236	CA	MET	D	34	95.230	38.000	53.378	1.00	11.29		C
ANISOU14236	CA	MET	D	34	1202	1496	1588	-19	22	97	C
ATOM 14238	CB	MET	D	34	95.389	39.530	53.360	1.00	12.61		C
ANISOU14238	CB	MET	D	34	1353	1658	1777	-34	31	53	C
ATOM 14241	CG	MET	D	34	94.482	40.438	52.315	1.00	14.19		C
ANISOU14241	CG	MET	D	34	1906	1784	1699	135	213	66	C
ATOM 14249	C	MET	D	34	95.563	37.380	52.048	1.00	11.30		C
ANISOU14249	C	MET	D	34	1245	1372	1675	-18	58	90	C
ATOM 14250	O	MET	D	34	94.689	37.200	51.247	1.00	9.38		O
ANISOU14250	O	MET	D	34	1217	1069	1276	174	121	396	O
ATOM 14251	N	ILE	D	35	96.850	37.004	51.799	1.00	12.32		N
ANISOU14251	N	ILE	D	35	1241	1669	1767	105	-9	109	N
ATOM 14253	CA	ILE	D	35	97.193	36.467	50.504	1.00	12.29		C
ANISOU14253	CA	ILE	D	35	1376	1601	1690	75	20	76	C
ATOM 14255	CB	ILE	D	35	98.770	36.389	50.341	1.00	13.91		C
ANISOU14255	CB	ILE	D	35	1567	1797	1920	98	-33	17	C
ATOM 14257	CG1	ILE	D	35	99.101	36.238	48.856	1.00	14.65		C
ANISOU14257	CG1	ILE	D	35	1693	1906	1964	70	88	-1	C

ATOM 14264	CG2	ILE	D	35	99.307	35.288	51.176	1.00	15.92		C
ANISOU14264	CG2	ILE	D	35	1905	2109	2034	68	1	49	C
ATOM 14268	C	ILE	D	35	96.498	35.168	50.153	1.00	11.67		C
ANISOU14268	C	ILE	D	35	1281	1606	1544	130	-14	99	C
ATOM 14269	O	ILE	D	35	96.377	34.790	48.972	1.00	10.70		O
ANISOU14269	O	ILE	D	35	1306	1447	1312	96	34	167	O
ATOM 14270	N	TYR	D	36	96.056	34.419	51.155	1.00	10.53		N
ANISOU14270	N	TYR	D	36	1161	1437	1403	60	5	89	N
ATOM 14272	CA	TYR	D	36	95.335	33.188	50.852	1.00	11.54		C
ANISOU14272	CA	TYR	D	36	1412	1519	1453	56	-25	78	C
ATOM 14274	CB	TYR	D	36	94.888	32.521	52.171	1.00	11.49		C
ANISOU14274	CB	TYR	D	36	1406	1593	1366	-43	-74	89	C
ATOM 14277	CG	TYR	D	36	95.908	31.654	52.876	1.00	12.21		C
ANISOU14277	CG	TYR	D	36	1504	1569	1566	51	63	120	C
ATOM 14278	CD1	TYR	D	36	97.247	31.865	52.716	1.00	12.64		C
ANISOU14278	CD1	TYR	D	36	1451	1692	1659	70	-75	76	C
ATOM 14280	CE1	TYR	D	36	98.190	31.099	53.386	1.00	13.00		C
ANISOU14280	CE1	TYR	D	36	1479	1670	1790	91	-17	175	C
ATOM 14282	CZ	TYR	D	36	97.782	30.131	54.245	1.00	13.08		C
ANISOU14282	CZ	TYR	D	36	1378	1705	1885	-11	23	104	C
ATOM 14283	OH	TYR	D	36	98.695	29.367	54.891	1.00	12.45		O
ANISOU14283	OH	TYR	D	36	1423	1994	1314	-109	109	304	O
ATOM 14285	CE2	TYR	D	36	96.417	29.877	54.435	1.00	12.76		C
ANISOU14285	CE2	TYR	D	36	1334	1814	1697	-23	42	138	C
ATOM 14287	CD2	TYR	D	36	95.489	30.661	53.753	1.00	13.60		C
ANISOU14287	CD2	TYR	D	36	1973	1556	1637	74	-52	47	C
ATOM 14289	C	TYR	D	36	94.043	33.425	49.992	1.00	9.82		C
ANISOU14289	C	TYR	D	36	1073	1374	1282	0	88	88	C
ATOM 14290	O	TYR	D	36	93.612	32.557	49.234	1.00	9.73		O
ANISOU14290	O	TYR	D	36	1007	1517	1172	349	55	73	O
ATOM 14291	N	TYR	D	37	93.488	34.634	50.087	1.00	10.75		N
ANISOU14291	N	TYR	D	37	1263	1477	1342	-21	112	39	N
ATOM 14293	CA	TYR	D	37	92.214	34.958	49.455	1.00	10.89		C
ANISOU14293	CA	TYR	D	37	1362	1395	1379	48	47	65	C
ATOM 14295	CB	TYR	D	37	91.522	36.136	50.133	1.00	11.33		C
ANISOU14295	CB	TYR	D	37	1499	1499	1306	2	19	5	C
ATOM 14298	CG	TYR	D	37	91.108	35.805	51.562	1.00	9.88		C
ANISOU14298	CG	TYR	D	37	1326	1195	1230	25	52	28	C
ATOM 14299	CD1	TYR	D	37	91.979	35.991	52.618	1.00	9.15		C
ANISOU14299	CD1	TYR	D	37	963	1372	1141	-54	108	20	C
ATOM 14301	CE1	TYR	D	37	91.598	35.659	53.937	1.00	7.73		C
ANISOU14301	CE1	TYR	D	37	762	1146	1028	24	55	-40	C
ATOM 14303	CZ	TYR	D	37	90.377	35.137	54.177	1.00	9.03		C
ANISOU14303	CZ	TYR	D	37	1233	1163	1033	-129	-10	-79	C
ATOM 14304	OH	TYR	D	37	90.044	34.798	55.489	1.00	7.85		O
ANISOU14304	OH	TYR	D	37	1242	879	860	-229	-210	103	O
ATOM 14306	CE2	TYR	D	37	89.471	34.933	53.125	1.00	9.02		C
ANISOU14306	CE2	TYR	D	37	996	1165	1265	144	-68	56	C
ATOM 14308	CD2	TYR	D	37	89.838	35.259	51.845	1.00	9.07		C
ANISOU14308	CD2	TYR	D	37	1152	1144	1148	120	-118	-10	C
ATOM 14310	C	TYR	D	37	92.421	35.100	47.961	1.00	10.54		C
ANISOU14310	C	TYR	D	37	1242	1428	1334	132	90	92	C
ATOM 14311	O	TYR	D	37	91.931	34.316	47.193	1.00	10.33		O
ANISOU14311	O	TYR	D	37	924	1491	1508	125	200	156	O
ATOM 14312	N	PRO	D	38	93.240	36.017	47.532	1.00	11.44		N
ANISOU14312	N	PRO	D	38	1441	1449	1454	149	39	38	N
ATOM 14313	CA	PRO	D	38	93.554	36.040	46.089	1.00	11.86		C
ANISOU14313	CA	PRO	D	38	1554	1535	1417	17	61	74	C
ATOM 14315	CB	PRO	D	38	94.448	37.255	45.967	1.00	12.13		C
ANISOU14315	CB	PRO	D	38	1448	1589	1570	26	5	6	C
ATOM 14318	CG	PRO	D	38	94.935	37.510	47.318	1.00	13.55		C

ANISOU14318	CG	PRO	D	38	1789	1690	1669	73	79	62	C
ATOM 14321	CD	PRO	D	38	93.852	37.147	48.241	1.00	12.23		C
ANISOU14321	CD	PRO	D	38	1475	1696	1475	76	32	93	C
ATOM 14324	C	PRO	D	38	94.220	34.753	45.543	1.00	10.91		C
ANISOU14324	C	PRO	D	38	1358	1477	1310	-24	73	86	C
ATOM 14325	O	PRO	D	38	94.004	34.350	44.388	1.00	10.09		O
ANISOU14325	O	PRO	D	38	1382	1300	1151	-256	138	256	O
ATOM 14326	N	LEU	D	39	95.026	34.089	46.352	1.00	11.37		N
ANISOU14326	N	LEU	D	39	1533	1489	1297	-39	119	98	N
ATOM 14328	CA	LEU	D	39	95.603	32.814	45.930	1.00	11.05		C
ANISOU14328	CA	LEU	D	39	1456	1499	1241	-19	122	114	C
ATOM 14330	CB	LEU	D	39	96.607	32.295	46.964	1.00	11.17		C
ANISOU14330	CB	LEU	D	39	1423	1450	1371	32	114	-6	C
ATOM 14333	CG	LEU	D	39	97.095	30.880	46.629	1.00	12.36		C
ANISOU14333	CG	LEU	D	39	1555	1521	1617	67	51	24	C
ATOM 14335	CD1	LEU	D	39	97.993	30.865	45.380	1.00	15.12		C
ANISOU14335	CD1	LEU	D	39	1956	1943	1843	133	126	23	C
ATOM 14339	CD2	LEU	D	39	97.844	30.371	47.797	1.00	12.75		C
ANISOU14339	CD2	LEU	D	39	1810	1521	1512	285	82	-106	C
ATOM 14343	C	LEU	D	39	94.481	31.790	45.614	1.00	11.37		C
ANISOU14343	C	LEU	D	39	1542	1466	1312	-37	101	138	C
ATOM 14344	O	LEU	D	39	94.504	31.112	44.567	1.00	11.62		O
ANISOU14344	O	LEU	D	39	1642	1586	1187	-194	360	337	O
ATOM 14345	N	SER	D	40	93.478	31.691	46.510	1.00	10.55		N
ANISOU14345	N	SER	D	40	1326	1462	1218	36	18	83	N
ATOM 14347	CA	SER	D	40	92.364	30.785	46.311	1.00	11.33		C
ANISOU14347	CA	SER	D	40	1398	1496	1410	35	60	114	C
ATOM 14349	CB	SER	D	40	91.389	30.798	47.524	1.00	11.65		C
ANISOU14349	CB	SER	D	40	1377	1674	1373	-4	54	59	C
ATOM 14352	OG	SER	D	40	90.555	31.978	47.533	1.00	12.46		O
ANISOU14352	OG	SER	D	40	1482	1854	1398	-110	470	-84	O
ATOM 14354	C	SER	D	40	91.594	31.122	45.045	1.00	10.33		C
ANISOU14354	C	SER	D	40	1080	1485	1360	69	39	35	C
ATOM 14355	O	SER	D	40	91.125	30.217	44.332	1.00	10.96		O
ANISOU14355	O	SER	D	40	682	1795	1684	240	12	136	O
ATOM 14356	N	THR	D	41	91.524	32.416	44.741	1.00	9.61		N
ANISOU14356	N	THR	D	41	926	1362	1363	37	18	88	N
ATOM 14358	CA	THR	D	41	90.828	32.822	43.548	1.00	10.81		C
ANISOU14358	CA	THR	D	41	1326	1400	1379	-59	35	55	C
ATOM 14360	CB	THR	D	41	90.734	34.359	43.467	1.00	11.27		C
ANISOU14360	CB	THR	D	41	1353	1494	1434	87	-6	-6	C
ATOM 14362	OG1	THR	D	41	89.828	34.828	44.474	1.00	12.66		O
ANISOU14362	OG1	THR	D	41	1444	1901	1462	121	124	-92	O
ATOM 14364	CG2	THR	D	41	90.174	34.798	42.119	1.00	10.27		C
ANISOU14364	CG2	THR	D	41	1238	1188	1475	-31	-138	-148	C
ATOM 14368	C	THR	D	41	91.490	32.248	42.286	1.00	11.57		C
ANISOU14368	C	THR	D	41	1481	1484	1432	-11	-28	7	C
ATOM 14369	O	THR	D	41	90.798	31.707	41.413	1.00	11.54		O
ANISOU14369	O	THR	D	41	1323	1689	1373	-208	-200	120	O
ATOM 14370	N	LEU	D	42	92.804	32.380	42.179	1.00	10.14		N
ANISOU14370	N	LEU	D	42	1296	1329	1225	-81	-38	93	N
ATOM 14372	CA	LEU	D	42	93.507	31.756	41.077	1.00	11.90		C
ANISOU14372	CA	LEU	D	42	1534	1517	1467	-3	6	21	C
ATOM 14374	CB	LEU	D	42	94.961	32.086	41.121	1.00	12.05		C
ANISOU14374	CB	LEU	D	42	1580	1601	1397	-103	54	-37	C
ATOM 14377	CG	LEU	D	42	95.224	33.574	40.884	1.00	14.25		C
ANISOU14377	CG	LEU	D	42	1949	1667	1797	41	-125	-38	C
ATOM 14379	CD1	LEU	D	42	96.731	33.752	40.860	1.00	14.05		C
ANISOU14379	CD1	LEU	D	42	1853	1795	1687	-31	59	-31	C
ATOM 14383	CD2	LEU	D	42	94.647	34.164	39.610	1.00	14.01		C
ANISOU14383	CD2	LEU	D	42	1785	1827	1709	88	-41	-58	C

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ATOM 14387	C	LEU D	42	93.348	30.238	41.042	1.00	11.79		C
ANISOU14387	C	LEU D	42	1437	1539	1503	25	113	-1	C
ATOM 14388	O	LEU D	42	93.024	29.683	40.011	1.00	12.62		O
ANISOU14388	O	LEU D	42	1540	1629	1626	35	157	-28	O
ATOM 14389	N	MET D	43	93.463	29.592	42.186	1.00	12.35		N
ANISOU14389	N	MET D	43	1401	1569	1720	124	-7	14	N
ATOM 14391	CA	MET D	43	93.224	28.151	42.264	1.00	11.81		C
ANISOU14391	CA	MET D	43	1436	1489	1562	31	15	-38	C
ATOM 14393	CB	MET D	43	93.398	27.702	43.702	1.00	12.98		C
ANISOU14393	CB	MET D	43	1572	1591	1768	99	-69	-39	C
ATOM 14396	CG	MET D	43	94.863	27.795	44.195	1.00	12.17		C
ANISOU14396	CG	MET D	43	1384	1467	1773	88	21	-126	C
ATOM 14399	SD	MET D	43	95.078	27.432	45.997	1.00	12.56		S
ANISOU14399	SD	MET D	43	1500	1546	1723	325	323	-100	S
ATOM 14400	CE	MET D	43	94.788	25.680	45.995	1.00	14.32		C
ANISOU14400	CE	MET D	43	1713	1921	1805	-49	71	-58	C
ATOM 14404	C	MET D	43	91.821	27.756	41.754	1.00	12.65		C
ANISOU14404	C	MET D	43	1624	1594	1588	0	0	-44	C
ATOM 14405	O	MET D	43	91.681	26.776	40.996	1.00	11.64		O
ANISOU14405	O	MET D	43	1463	1536	1421	12	-89	-127	O
ATOM 14406	N	LEU D	44	90.792	28.483	42.174	1.00	12.15		N
ANISOU14406	N	LEU D	44	1504	1519	1591	27	31	24	N
ATOM 14408	CA	LEU D	44	89.438	28.181	41.725	1.00	14.17		C
ANISOU14408	CA	LEU D	44	1786	1810	1787	47	-29	-15	C
ATOM 14410	CB	LEU D	44	88.398	28.938	42.557	1.00	14.07		C
ANISOU14410	CB	LEU D	44	1803	1727	1813	80	14	-92	C
ATOM 14413	CG	LEU D	44	88.320	28.494	44.013	1.00	15.62		C
ANISOU14413	CG	LEU D	44	1956	1933	2045	104	-48	3	C
ATOM 14415	CD1	LEU D	44	87.620	29.556	44.902	1.00	19.16		C
ANISOU14415	CD1	LEU D	44	2471	2397	2410	59	105	10	C
ATOM 14419	CD2	LEU D	44	87.616	27.172	44.105	1.00	16.73		C
ANISOU14419	CD2	LEU D	44	1810	2280	2266	-21	-2	139	C
ATOM 14423	C	LEU D	44	89.221	28.401	40.253	1.00	14.05		C
ANISOU14423	C	LEU D	44	1760	1841	1736	-36	13	-63	C
ATOM 14424	O	LEU D	44	88.272	27.842	39.660	1.00	15.74		O
ANISOU14424	O	LEU D	44	1838	2231	1909	-111	38	-70	O
ATOM 14425	N	ALA D	45	90.052	29.238	39.666	1.00	13.84		N
ANISOU14425	N	ALA D	45	1652	1888	1717	15	-51	-135	N
ATOM 14427	CA	ALA D	45	90.095	29.436	38.231	1.00	13.52		C
ANISOU14427	CA	ALA D	45	1645	1800	1690	-26	-33	-33	C
ATOM 14429	CB	ALA D	45	90.722	30.723	37.905	1.00	13.79		C
ANISOU14429	CB	ALA D	45	1764	1808	1667	21	-25	-85	C
ATOM 14433	C	ALA D	45	90.829	28.290	37.529	1.00	13.47		C
ANISOU14433	C	ALA D	45	1567	1854	1696	-25	-6	-27	C
ATOM 14434	O	ALA D	45	90.907	28.281	36.303	1.00	13.33		O
ANISOU14434	O	ALA D	45	1442	2011	1611	-57	156	-126	O
ATOM 14435	N	GLY D	46	91.348	27.324	38.283	1.00	13.27		N
ANISOU14435	N	GLY D	46	1613	1769	1660	-41	26	-30	N
ATOM 14437	CA	GLY D	46	92.076	26.209	37.686	1.00	14.31		C
ANISOU14437	CA	GLY D	46	1714	1818	1903	-14	-58	0	C
ATOM 14440	C	GLY D	46	93.567	26.464	37.423	1.00	14.09		C
ANISOU14440	C	GLY D	46	1757	1797	1799	14	18	28	C
ATOM 14441	O	GLY D	46	94.202	25.684	36.735	1.00	14.78		O
ANISOU14441	O	GLY D	46	1912	1843	1861	-34	-51	-38	O
ATOM 14442	N	ILE D	47	94.121	27.532	37.986	1.00	13.28		N
ANISOU14442	N	ILE D	47	1643	1715	1686	-34	-31	-3	N
ATOM 14444	CA	ILE D	47	95.511	27.931	37.756	1.00	12.54		C
ANISOU14444	CA	ILE D	47	1570	1679	1515	50	-18	18	C
ATOM 14446	CB	ILE D	47	95.581	29.455	37.672	1.00	11.95		C
ANISOU14446	CB	ILE D	47	1504	1666	1367	-31	-39	4	C
ATOM 14448	CG1	ILE D	47	94.725	29.937	36.494	1.00	12.13		C

ANISOU14448	CG1	ILE	D	47	1416	1645	1547	60	-35	42	C
ATOM 14451	CD1	ILE	D	47	94.571	31.426	36.407	1.00	11.78		C
ANISOU14451	CD1	ILE	D	47	1567	1547	1360	-185	14	32	C
ATOM 14459	C	ILE	D	47	96.357	27.397	38.887	1.00	13.58		C
ANISOU14459	C	ILE	D	47	1697	1801	1662	-20	-25	8	C
ATOM 14460	O	ILE	D	47	96.023	27.593	40.045	1.00	14.57		O
ANISOU14460	O	ILE	D	47	1697	2032	1806	53	-119	-22	O
ATOM 14461	N	ARG	D	48	97.367	26.627	38.517	1.00	13.04		N
ANISOU14461	N	ARG	D	48	1568	1704	1680	-8	-7	55	N
ATOM 14463	CA	ARG	D	48	98.299	26.013	39.431	1.00	13.81		C
ANISOU14463	CA	ARG	D	48	1701	1811	1732	-3	-8	40	C
ATOM 14468	CG	ARG	D	48	97.138	23.736	39.228	1.00	17.74		C
ANISOU14468	CG	ARG	D	48	2293	2205	2240	-49	3	70	C
ATOM 14471	CD	ARG	D	48	97.310	22.245	38.784	1.00	19.98		C
ANISOU14471	CD	ARG	D	48	2757	2326	2507	0	-81	18	C
ATOM 14474	NE	ARG	D	48	98.097	21.449	39.741	1.00	20.52		N
ANISOU14474	NE	ARG	D	48	2777	2439	2580	31	-67	74	N
ATOM 14509	CD1	ILE	D	50	98.520	30.073	41.872	1.00	11.36		C
ANISOU14509	CD1	ILE	D	50	1361	1303	1651	-109	-9	83	C
ATOM 14782	CD2	LEU	D	66	101.155	30.828	50.804	1.00	15.18		C
ANISOU14782	CD2	LEU	D	66	1649	1917	2200	207	143	-33	C
ATOM 14837	C	ASN	D	71	101.168	20.975	48.977	1.00	17.90		C
ANISOU14837	C	ASN	D	71	2274	2289	2238	5	54	-8	C
ATOM 14838	O	ASN	D	71	100.316	20.126	49.362	1.00	18.28		O
ANISOU14838	O	ASN	D	71	2384	2273	2286	-68	-6	-71	O
ATOM 14839	N	TRP	D	72	100.854	22.044	48.244	1.00	17.26		N
ANISOU14839	N	TRP	D	72	2187	2201	2167	-72	119	4	N
ATOM 14841	CA	TRP	D	72	99.504	22.295	47.805	1.00	16.86		C
ANISOU14841	CA	TRP	D	72	2191	2137	2075	-28	51	3	C
ATOM 14843	CB	TRP	D	72	99.123	23.750	48.040	1.00	16.48		C
ANISOU14843	CB	TRP	D	72	2112	2156	1994	-2	73	-47	C
ATOM 14846	CG	TRP	D	72	99.190	24.124	49.488	1.00	15.13		C
ANISOU14846	CG	TRP	D	72	1898	1927	1923	-78	-34	6	C
ATOM 14847	CD1	TRP	D	72	99.278	23.276	50.546	1.00	13.84		C
ANISOU14847	CD1	TRP	D	72	1668	1875	1715	-79	44	-53	C
ATOM 14849	NE1	TRP	D	72	99.312	23.986	51.718	1.00	12.36		N
ANISOU14849	NE1	TRP	D	72	1437	1669	1590	-53	-63	7	N
ATOM 14851	CE2	TRP	D	72	99.270	25.319	51.425	1.00	11.87		C
ANISOU14851	CE2	TRP	D	72	1335	1574	1599	111	66	32	C
ATOM 14852	CD2	TRP	D	72	99.194	25.434	50.023	1.00	12.19		C
ANISOU14852	CD2	TRP	D	72	1244	1680	1705	167	33	13	C
ATOM 14853	CE3	TRP	D	72	99.164	26.706	49.460	1.00	14.25		C
ANISOU14853	CE3	TRP	D	72	1868	1793	1751	-21	-3	107	C
ATOM 14855	CZ3	TRP	D	72	99.171	27.815	50.306	1.00	14.45		C
ANISOU14855	CZ3	TRP	D	72	1879	1878	1731	-65	-38	-14	C
ATOM 14857	CH2	TRP	D	72	99.273	27.661	51.704	1.00	13.79		C
ANISOU14857	CH2	TRP	D	72	1765	1779	1696	32	-7	17	C
ATOM 14859	CZ2	TRP	D	72	99.320	26.421	52.275	1.00	13.61		C
ANISOU14859	CZ2	TRP	D	72	1711	1703	1755	-129	46	5	C
ATOM 14861	C	TRP	D	72	99.238	21.939	46.351	1.00	17.41		C
ANISOU14861	C	TRP	D	72	2242	2207	2166	0	24	-36	C
ATOM 14862	O	TRP	D	72	98.186	22.278	45.837	1.00	17.58		O
ANISOU14862	O	TRP	D	72	2172	2428	2080	-86	89	-64	O
ATOM 14863	N	GLY	D	73	100.152	21.220	45.705	1.00	16.90		N
ANISOU14863	N	GLY	D	73	2155	2192	2074	-91	103	-27	N
ATOM 14865	CA	GLY	D	73	99.942	20.873	44.309	1.00	17.18		C
ANISOU14865	CA	GLY	D	73	2236	2094	2195	-106	-9	40	C
ATOM 14868	C	GLY	D	73	100.141	22.053	43.357	1.00	16.47		C
ANISOU14868	C	GLY	D	73	2163	2035	2059	-68	-61	68	C
ATOM 14869	O	GLY	D	73	99.595	22.045	42.261	1.00	17.24		O
ANISOU14869	O	GLY	D	73	2312	2056	2182	-182	-95	102	O

ATOM 14874	CB	LEU	D	74	100.612	25.492	43.754	1.00	12.75			C
ANISOU14874	CB	LEU	D	74	1568	1533	1742	59	34	30		C
ATOM 14877	CG	LEU	D	74	99.200	25.509	44.303	1.00	13.84			C
ANISOU14877	CG	LEU	D	74	1752	1700	1807	-44	1	28		C
ATOM 14879	CD1	LEU	D	74	99.057	26.722	45.201	1.00	14.22			C
ANISOU14879	CD1	LEU	D	74	1768	1807	1824	-68	137	-30		C
ATOM 14883	CD2	LEU	D	74	98.146	25.513	43.166	1.00	12.74			C
ANISOU14883	CD2	LEU	D	74	1677	1556	1607	36	51	103		C
ATOM 15339	CA	VAL	D	106	94.699	39.207	40.751	1.00	11.00			C
ANISOU15339	CA	VAL	D	106	1351	1469	1360	-6	-8	-2		C
ATOM 15341	CB	VAL	D	106	94.095	37.993	41.406	1.00	10.26			C
ANISOU15341	CB	VAL	D	106	1315	1292	1292	12	-21	-25		C
ATOM 15343	CG1	VAL	D	106	95.174	37.204	42.185	1.00	10.61			C
ANISOU15343	CG1	VAL	D	106	1560	1406	1061	162	34	-163		C
ATOM 15347	CG2	VAL	D	106	93.033	38.385	42.322	1.00	11.05			C
ANISOU15347	CG2	VAL	D	106	1341	1447	1407	163	-91	-18		C
ATOM 15371	O	LEU	D	107	94.438	40.815	45.072	1.00	12.14			O
ANISOU15371	O	LEU	D	107	1799	1652	1159	-146	-80	79		O
ATOM 15378	O	GLY	D	108	95.611	40.743	48.665	1.00	15.45			O
ANISOU15378	O	GLY	D	108	2006	1748	2117	-151	46	118		O
ATOM 15389	C	ASP	D	109	92.737	42.993	48.209	1.00	14.09			C
ANISOU15389	C	ASP	D	109	1805	1842	1706	27	-4	-8		C
ATOM 15390	O	ASP	D	109	91.856	43.593	48.833	1.00	16.25			O
ANISOU15390	O	ASP	D	109	2182	2346	1644	128	16	-193		O
ATOM 15391	N	ASN	D	110	92.489	42.247	47.124	1.00	12.84			N
ANISOU15391	N	ASN	D	110	1679	1629	1569	-49	38	-18		N
ATOM 15393	CA	ASN	D	110	91.113	41.982	46.647	1.00	12.22			C
ANISOU15393	CA	ASN	D	110	1509	1604	1528	48	28	40		C
ATOM 15395	CB	ASN	D	110	91.063	41.988	45.147	1.00	12.92			C
ANISOU15395	CB	ASN	D	110	1600	1685	1620	-54	59	-95		C
ATOM 15398	CG	ASN	D	110	90.983	43.393	44.533	1.00	13.15			C
ANISOU15398	CG	ASN	D	110	1680	1859	1457	-106	47	152		C
ATOM 15399	OD1	ASN	D	110	90.241	43.561	43.564	1.00	15.33			O
ANISOU15399	OD1	ASN	D	110	1450	2680	1693	35	87	50		O
ATOM 15400	ND2	ASN	D	110	91.784	44.388	45.034	1.00	9.69			N
ANISOU15400	ND2	ASN	D	110	1297	1664	720	79	-20	252		N
ATOM 15403	C	ASN	D	110	90.552	40.630	47.130	1.00	12.08			C
ANISOU15403	C	ASN	D	110	1454	1587	1547	-17	44	-18		C
ATOM 15404	O	ASN	D	110	91.189	39.602	46.986	1.00	11.77			O
ANISOU15404	O	ASN	D	110	1245	1667	1559	-140	115	168		O
ATOM 15405	N	LEU	D	111	89.368	40.639	47.737	1.00	11.50			N
ANISOU15405	N	LEU	D	111	1242	1524	1603	54	-41	47		N
ATOM 15407	CA	LEU	D	111	88.732	39.439	48.250	1.00	11.92			C
ANISOU15407	CA	LEU	D	111	1406	1594	1528	57	-62	-38		C
ATOM 15409	CB	LEU	D	111	88.543	39.623	49.744	1.00	11.97			C
ANISOU15409	CB	LEU	D	111	1338	1651	1559	-57	-63	-51		C
ATOM 15412	CG	LEU	D	111	88.240	38.385	50.519	1.00	15.46			C
ANISOU15412	CG	LEU	D	111	2063	1984	1827	20	-100	38		C
ATOM 15414	CD1	LEU	D	111	88.606	38.587	51.977	1.00	17.03			C
ANISOU15414	CD1	LEU	D	111	2399	2101	1971	-111	-42	-82		C
ATOM 15418	CD2	LEU	D	111	86.734	38.168	50.378	1.00	17.60			C
ANISOU15418	CD2	LEU	D	111	2212	2533	1941	-195	95	104		C
ATOM 15422	C	LEU	D	111	87.353	39.248	47.569	1.00	11.55			C
ANISOU15422	C	LEU	D	111	1369	1571	1447	-16	-15	-62		C
ATOM 15423	O	LEU	D	111	86.504	40.145	47.658	1.00	12.57			O
ANISOU15423	O	LEU	D	111	1554	1670	1549	16	-209	-107		O
ATOM 15424	N	TYR	D	112	87.175	38.128	46.882	1.00	9.99			N
ANISOU15424	N	TYR	D	112	1200	1303	1289	-50	48	53		N
ATOM 15426	CA	TYR	D	112	85.934	37.814	46.198	1.00	11.39			C
ANISOU15426	CA	TYR	D	112	1469	1432	1424	-27	-21	26		C
ATOM 15428	CB	TYR	D	112	86.201	37.324	44.760	1.00	10.85			C

ANISOU15428	CB	TYR	D	112	1340	1469	1310	27	10	58	C
ATOM 15431	CG	TYR	D	112	86.860	38.370	43.881	1.00	12.72		C
ANISOU15431	CG	TYR	D	112	1518	1642	1671	-61	-13	62	C
ATOM 15432	CD1	TYR	D	112	88.267	38.535	43.845	1.00	11.45		C
ANISOU15432	CD1	TYR	D	112	1223	1641	1486	-158	-30	-1	C
ATOM 15434	CE1	TYR	D	112	88.836	39.528	43.071	1.00	12.33		C
ANISOU15434	CE1	TYR	D	112	1455	1912	1318	128	21	37	C
ATOM 15436	CZ	TYR	D	112	88.059	40.297	42.237	1.00	14.31		C
ANISOU15436	CZ	TYR	D	112	1649	1786	2002	132	81	191	C
ATOM 15437	OH	TYR	D	112	88.635	41.269	41.435	1.00	11.73		O
ANISOU15437	OH	TYR	D	112	1294	1571	1590	-39	223	-33	O
ATOM 15439	CE2	TYR	D	112	86.695	40.102	42.207	1.00	13.93		C
ANISOU15439	CE2	TYR	D	112	1697	1656	1937	16	-9	90	C
ATOM 15441	CD2	TYR	D	112	86.108	39.144	43.034	1.00	13.84		C
ANISOU15441	CD2	TYR	D	112	1398	1995	1865	19	9	141	C
ATOM 15443	C	TYR	D	112	85.232	36.671	46.923	1.00	11.25		C
ANISOU15443	C	TYR	D	112	1326	1509	1440	-68	26	96	C
ATOM 15444	O	TYR	D	112	85.893	35.760	47.431	1.00	9.95		O
ANISOU15444	O	TYR	D	112	1104	1465	1210	-232	-110	207	O
ATOM 15445	N	TYR	D	113	83.905	36.660	46.864	1.00	11.44		N
ANISOU15445	N	TYR	D	113	1439	1465	1441	55	-123	43	N
ATOM 15447	CA	TYR	D	113	83.136	35.565	47.420	1.00	10.77		C
ANISOU15447	CA	TYR	D	113	1166	1525	1399	-23	-64	38	C
ATOM 15449	CB	TYR	D	113	83.074	35.645	48.934	1.00	11.10		C
ANISOU15449	CB	TYR	D	113	1223	1471	1521	-58	-4	-27	C
ATOM 15452	CG	TYR	D	113	82.595	34.322	49.535	1.00	10.43		C
ANISOU15452	CG	TYR	D	113	1313	1169	1479	-120	-79	-109	C
ATOM 15453	CD1	TYR	D	113	83.468	33.317	49.753	1.00	9.29		C
ANISOU15453	CD1	TYR	D	113	1131	1227	1170	-75	-71	95	C
ATOM 15455	CE1	TYR	D	113	83.048	32.051	50.219	1.00	10.49		C
ANISOU15455	CE1	TYR	D	113	1289	1333	1364	-89	-263	220	C
ATOM 15457	CZ	TYR	D	113	81.721	31.851	50.533	1.00	11.89		C
ANISOU15457	CZ	TYR	D	113	1560	1584	1373	2	48	128	C
ATOM 15458	OH	TYR	D	113	81.374	30.595	50.988	1.00	13.39		O
ANISOU15458	OH	TYR	D	113	1555	1869	1661	-244	134	-14	O
ATOM 15460	CE2	TYR	D	113	80.824	32.882	50.318	1.00	10.41		C
ANISOU15460	CE2	TYR	D	113	1452	1232	1270	-138	9	-109	C
ATOM 15462	CD2	TYR	D	113	81.297	34.114	49.819	1.00	8.42		C
ANISOU15462	CD2	TYR	D	113	1228	1140	829	109	301	-275	C
ATOM 15464	C	TYR	D	113	81.712	35.466	46.863	1.00	10.45		C
ANISOU15464	C	TYR	D	113	1270	1430	1268	54	21	33	C
ATOM 15465	O	TYR	D	113	81.007	36.453	46.824	1.00	8.60		O
ANISOU15465	O	TYR	D	113	928	1216	1120	247	-232	30	O
ATOM 15466	N	GLY	D	114	81.321	34.277	46.451	1.00	9.07		N
ANISOU15466	N	GLY	D	114	1061	1236	1146	85	96	-59	N
ATOM 15468	CA	GLY	D	114	79.930	34.028	46.232	1.00	9.92		C
ANISOU15468	CA	GLY	D	114	1300	1265	1201	-21	-46	17	C
ATOM 15471	C	GLY	D	114	79.602	32.782	45.492	1.00	9.45		C
ANISOU15471	C	GLY	D	114	1221	1187	1180	31	-29	-10	C
ATOM 15472	O	GLY	D	114	80.498	32.064	45.067	1.00	8.37		O
ANISOU15472	O	GLY	D	114	845	1393	939	-72	-32	-203	O
ATOM 15473	N	HIS	D	115	78.294	32.576	45.333	1.00	8.61		N
ANISOU15473	N	HIS	D	115	1040	1134	1097	96	-46	44	N
ATOM 15475	CA	HIS	D	115	77.731	31.385	44.699	1.00	8.42		C
ANISOU15475	CA	HIS	D	115	967	1155	1074	59	-58	-16	C
ATOM 15477	CB	HIS	D	115	76.191	31.289	44.865	1.00	9.01		C
ANISOU15477	CB	HIS	D	115	1136	1291	996	-16	63	-37	C
ATOM 15480	CG	HIS	D	115	75.597	30.123	44.126	1.00	7.23		C
ANISOU15480	CG	HIS	D	115	699	907	1141	16	156	49	C
ATOM 15481	ND1	HIS	D	115	75.952	28.807	44.399	1.00	6.20		N
ANISOU15481	ND1	HIS	D	115	1019	622	713	111	182	-40	N

ATOM 15483	CE1	HIS	D	115	75.263	28.004	43.615	1.00	7.81		C
ANISOU15483	CE1	HIS	D	115	948	855	1162	126	20	-18	C
ATOM 15485	NE2	HIS	D	115	74.427	28.727	42.890	1.00	5.41		N
ANISOU15485	NE2	HIS	D	115	712	561	781	304	307	18	N
ATOM 15487	CD2	HIS	D	115	74.679	30.062	43.137	1.00	8.28		C
ANISOU15487	CD2	HIS	D	115	1326	718	1101	116	-100	29	C
ATOM 15489	C	HIS	D	115	78.109	31.325	43.235	1.00	8.57		C
ANISOU15489	C	HIS	D	115	1036	1184	1035	17	-95	-21	C
ATOM 15490	O	HIS	D	115	77.961	32.316	42.490	1.00	9.04		O
ANISOU15490	O	HIS	D	115	1181	1121	1129	-65	7	-186	O
ATOM 15491	N	ASP	D	116	78.714	30.190	42.872	1.00	9.73		N
ANISOU15491	N	ASP	D	116	1280	1334	1080	-113	-62	44	N
ATOM 15493	CA	ASP	D	116	79.116	29.893	41.522	1.00	10.85		C
ANISOU15493	CA	ASP	D	116	1380	1380	1361	-5	-33	-53	C
ATOM 15495	CB	ASP	D	116	77.854	29.934	40.640	1.00	10.53		C
ANISOU15495	CB	ASP	D	116	1238	1454	1308	58	-116	-49	C
ATOM 15498	CG	ASP	D	116	77.076	28.609	40.625	1.00	14.06		C
ANISOU15498	CG	ASP	D	116	1784	1810	1749	-64	-63	95	C
ATOM 15499	OD1	ASP	D	116	77.291	27.702	41.478	1.00	13.77		O
ANISOU15499	OD1	ASP	D	116	1653	1897	1682	189	31	-89	O
ATOM 15500	OD2	ASP	D	116	76.166	28.378	39.780	1.00	15.52		O
ANISOU15500	OD2	ASP	D	116	1849	2164	1883	-166	-257	423	O
ATOM 15501	C	ASP	D	116	80.253	30.828	41.005	1.00	10.86		C
ANISOU15501	C	ASP	D	116	1370	1369	1386	47	12	36	C
ATOM 15502	O	ASP	D	116	80.401	31.056	39.797	1.00	10.52		O
ANISOU15502	O	ASP	D	116	1353	1345	1300	165	-67	97	O
ATOM 15503	N	PHE	D	117	81.055	31.356	41.931	1.00	11.53		N
ANISOU15503	N	PHE	D	117	1380	1472	1525	71	-2	50	N
ATOM 15505	CA	PHE	D	117	82.303	32.073	41.560	1.00	12.16		C
ANISOU15505	CA	PHE	D	117	1535	1509	1574	-32	-10	44	C
ATOM 15507	CB	PHE	D	117	83.034	32.528	42.824	1.00	12.57		C
ANISOU15507	CB	PHE	D	117	1586	1577	1613	48	-10	-31	C
ATOM 15510	CG	PHE	D	117	84.206	33.470	42.591	1.00	11.44		C
ANISOU15510	CG	PHE	D	117	1417	1541	1387	44	-34	-110	C
ATOM 15511	CD1	PHE	D	117	84.115	34.557	41.742	1.00	13.84		C
ANISOU15511	CD1	PHE	D	117	1687	1715	1854	-2	-149	-103	C
ATOM 15513	CE1	PHE	D	117	85.155	35.432	41.529	1.00	14.37		C
ANISOU15513	CE1	PHE	D	117	1689	1756	2012	101	87	120	C
ATOM 15515	CZ	PHE	D	117	86.353	35.237	42.175	1.00	14.26		C
ANISOU15515	CZ	PHE	D	117	1740	1941	1736	-119	-37	85	C
ATOM 15517	CE2	PHE	D	117	86.466	34.170	43.098	1.00	14.03		C
ANISOU15517	CE2	PHE	D	117	1665	1595	2068	29	70	-65	C
ATOM 15519	CD2	PHE	D	117	85.379	33.286	43.293	1.00	11.27		C
ANISOU15519	CD2	PHE	D	117	1312	1601	1368	117	81	-63	C
ATOM 15521	C	PHE	D	117	83.218	31.153	40.731	1.00	12.53		C
ANISOU15521	C	PHE	D	117	1515	1605	1641	-8	-91	34	C
ATOM 15522	O	PHE	D	117	83.913	31.619	39.778	1.00	13.20		O
ANISOU15522	O	PHE	D	117	1826	1522	1664	120	2	115	O
ATOM 15523	N	HIS	D	118	83.247	29.852	41.060	1.00	13.03		N
ANISOU15523	N	HIS	D	118	1625	1671	1651	-13	-97	57	N
ATOM 15525	CA	HIS	D	118	84.098	28.947	40.308	1.00	14.31		C
ANISOU15525	CA	HIS	D	118	1829	1814	1793	22	-47	56	C
ATOM 15527	CB	HIS	D	118	84.237	27.562	40.982	1.00	16.00		C
ANISOU15527	CB	HIS	D	118	2063	2038	1977	-34	111	100	C
ATOM 15530	CG	HIS	D	118	83.217	26.570	40.606	1.00	20.20		C
ANISOU15530	CG	HIS	D	118	2584	2583	2507	-64	-209	35	C
ATOM 15531	ND1	HIS	D	118	82.350	26.076	41.566	1.00	24.31		N
ANISOU15531	ND1	HIS	D	118	2958	3220	3056	29	158	-62	N
ATOM 15533	CE1	HIS	D	118	81.667	25.066	41.058	1.00	23.57		C
ANISOU15533	CE1	HIS	D	118	2980	2872	3104	36	-83	-16	C
ATOM 15535	NE2	HIS	D	118	82.141	24.823	39.845	1.00	25.04		N

ANISOU15535	NE2	HIS	D	118	3038	3145	3331	-64	74	-28	N
ATOM 15537	CD2	HIS	D	118	83.242	25.627	39.633	1.00	23.54		C
ANISOU15537	CD2	HIS	D	118	3066	2815	3061	93	56	-150	C
ATOM 15539	C	HIS	D	118	83.711	28.869	38.832	1.00	13.65		C
ANISOU15539	C	HIS	D	118	1723	1704	1758	-49	32	-9	C
ATOM 15540	O	HIS	D	118	84.580	28.796	37.966	1.00	14.09		O
ANISOU15540	O	HIS	D	118	1815	1752	1784	-208	122	48	O
ATOM 15541	N	GLU	D	119	82.420	28.913	38.546	1.00	13.44		N
ANISOU15541	N	GLU	D	119	1740	1611	1754	-11	4	53	N
ATOM 15543	CA	GLU	D	119	81.967	28.860	37.190	1.00	13.71		C
ANISOU15543	CA	GLU	D	119	1716	1787	1704	-28	32	42	C
ATOM 15545	CB	GLU	D	119	80.436	28.531	37.079	1.00	14.49		C
ANISOU15545	CB	GLU	D	119	1784	1889	1832	-78	32	8	C
ATOM 15548	CG	GLU	D	119	80.031	27.092	37.448	1.00	14.57		C
ANISOU15548	CG	GLU	D	119	1980	1825	1730	-38	96	-38	C
ATOM 15551	CD	GLU	D	119	79.727	26.813	38.925	1.00	15.51		C
ANISOU15551	CD	GLU	D	119	2224	1888	1780	-131	-50	-27	C
ATOM 15552	OE1	GLU	D	119	80.083	27.614	39.789	1.00	12.17		O
ANISOU15552	OE1	GLU	D	119	2148	897	1577	-147	-68	188	O
ATOM 15553	OE2	GLU	D	119	79.147	25.709	39.215	1.00	16.54		O
ANISOU15553	OE2	GLU	D	119	2091	2122	2071	-91	199	53	O
ATOM 15554	C	GLU	D	119	82.230	30.194	36.498	1.00	13.46		C
ANISOU15554	C	GLU	D	119	1656	1713	1744	-105	60	41	C
ATOM 15555	O	GLU	D	119	82.547	30.213	35.305	1.00	11.96		O
ANISOU15555	O	GLU	D	119	1358	1594	1589	-150	179	251	O
ATOM 15556	N	LEU	D	120	82.025	31.293	37.203	1.00	14.15		N
ANISOU15556	N	LEU	D	120	1739	1829	1806	-145	110	143	N
ATOM 15558	CA	LEU	D	120	82.307	32.621	36.624	1.00	14.37		C
ANISOU15558	CA	LEU	D	120	1837	1825	1796	-29	-53	138	C
ATOM 15560	CB	LEU	D	120	82.044	33.677	37.687	1.00	15.13		C
ANISOU15560	CB	LEU	D	120	1866	1956	1927	52	-25	128	C
ATOM 15563	CG	LEU	D	120	82.489	35.101	37.419	1.00	17.51		C
ANISOU15563	CG	LEU	D	120	2353	2133	2165	-23	65	73	C
ATOM 15565	CD1	LEU	D	120	81.801	35.366	36.137	1.00	21.59		C
ANISOU15565	CD1	LEU	D	120	2897	2609	2697	-66	-126	152	C
ATOM 15569	CD2	LEU	D	120	82.082	36.143	38.461	1.00	17.90		C
ANISOU15569	CD2	LEU	D	120	2448	1995	2356	20	-209	115	C
ATOM 15573	C	LEU	D	120	83.796	32.670	36.191	1.00	14.11		C
ANISOU15573	C	LEU	D	120	1763	1858	1738	23	89	125	C
ATOM 15574	O	LEU	D	120	84.175	33.222	35.106	1.00	13.11		O
ANISOU15574	O	LEU	D	120	1653	1714	1614	-65	1	185	O
ATOM 15575	N	LEU	D	121	84.671	32.114	37.036	1.00	13.04		N
ANISOU15575	N	LEU	D	121	1603	1731	1621	-20	83	114	N
ATOM 15577	CA	LEU	D	121	86.121	32.130	36.700	1.00	13.96		C
ANISOU15577	CA	LEU	D	121	1727	1827	1747	26	96	31	C
ATOM 15579	CB	LEU	D	121	86.982	31.692	37.870	1.00	13.46		C
ANISOU15579	CB	LEU	D	121	1595	1853	1663	36	70	5	C
ATOM 15582	CG	LEU	D	121	86.897	32.647	39.089	1.00	13.40		C
ANISOU15582	CG	LEU	D	121	1523	1647	1918	9	-140	6	C
ATOM 15584	CD1	LEU	D	121	87.216	31.984	40.395	1.00	14.50		C
ANISOU15584	CD1	LEU	D	121	1815	1771	1922	-212	69	46	C
ATOM 15588	CD2	LEU	D	121	87.777	33.872	38.859	1.00	13.43		C
ANISOU15588	CD2	LEU	D	121	1676	1664	1760	-73	-32	43	C
ATOM 15592	C	LEU	D	121	86.397	31.208	35.516	1.00	15.37		C
ANISOU15592	C	LEU	D	121	1957	1982	1898	-13	101	16	C
ATOM 15593	O	LEU	D	121	87.192	31.553	34.623	1.00	13.73		O
ANISOU15593	O	LEU	D	121	1786	1707	1723	81	353	-125	O
ATOM 15594	N	GLY	D	122	85.777	30.020	35.543	1.00	16.28		N
ANISOU15594	N	GLY	D	122	2189	1944	2052	-8	114	-17	N
ATOM 15596	CA	GLY	D	122	85.896	29.069	34.458	1.00	18.89		C
ANISOU15596	CA	GLY	D	122	2468	2354	2355	-40	17	-28	C

ATOM 15599	C	GLY D 122	85.479	29.662	33.143	1.00	19.26		C
ANISOU15599	C	GLY D 122	2522	2383	2410	-68	28	-17	C
ATOM 15600	O	GLY D 122	86.164	29.507	32.139	1.00	20.50		O
ANISOU15600	O	GLY D 122	2663	2572	2550	-129	119	-192	O
ATOM 15601	N	SER D 123	84.356	30.340	33.126	1.00	18.95		N
ANISOU15601	N	SER D 123	2358	2407	2436	-125	90	-44	N
ATOM 15603	CA	SER D 123	83.947	30.974	31.900	1.00	20.93		C
ANISOU15603	CA	SER D 123	2625	2647	2679	-79	-4	-37	C
ATOM 15605	CB	SER D 123	82.592	31.598	32.093	1.00	21.46		C
ANISOU15605	CB	SER D 123	2641	2731	2780	-79	38	18	C
ATOM 15608	OG	SER D 123	81.743	30.528	32.486	1.00	23.87		O
ANISOU15608	OG	SER D 123	2974	2901	3192	-235	93	82	O
ATOM 15610	C	SER D 123	84.965	31.989	31.377	1.00	20.92		C
ANISOU15610	C	SER D 123	2605	2754	2586	-97	22	-21	C
ATOM 15611	O	SER D 123	85.218	32.042	30.167	1.00	21.68		O
ANISOU15611	O	SER D 123	2734	3005	2495	-107	-187	-195	O
ATOM 15612	N	ALA D 124	85.562	32.799	32.258	1.00	19.51		N
ANISOU15612	N	ALA D 124	2532	2502	2377	-81	41	-73	N
ATOM 15614	CA	ALA D 124	86.543	33.747	31.760	1.00	19.42		C
ANISOU15614	CA	ALA D 124	2537	2471	2370	-51	-34	-20	C
ATOM 15616	CB	ALA D 124	86.844	34.884	32.793	1.00	19.42		C
ANISOU15616	CB	ALA D 124	2594	2416	2365	-15	54	-24	C
ATOM 15620	C	ALA D 124	87.819	33.050	31.369	1.00	19.74		C
ANISOU15620	C	ALA D 124	2617	2467	2416	-63	35	-79	C
ATOM 15622	N	SER D 125	88.225	32.025	32.095	1.00	21.12		N
ANISOU15622	N	SER D 125	2781	2704	2540	-36	9	-55	N
ATOM 15624	CA	SER D 125	89.490	31.390	31.774	1.00	23.17		C
ANISOU15624	CA	SER D 125	2945	2936	2923	-33	21	-25	C
ATOM 15626	CB	SER D 125	89.961	30.500	32.920	1.00	24.07		C
ANISOU15626	CB	SER D 125	3117	3040	2987	-59	-38	24	C
ATOM 15629	OG	SER D 125	89.514	29.173	32.774	1.00	26.65		O
ANISOU15629	OG	SER D 125	3387	3443	3296	-24	-194	-92	O
ATOM 15633	N	GLN D 126	88.277	30.268	30.005	1.00	26.06		N
ANISOU15633	N	GLN D 126	3314	3329	3256	-78	61	-26	N
ATOM 15640	CG	GLN D 126	87.309	27.336	29.576	1.00	32.72		C
ANISOU15640	CG	GLN D 126	4227	4092	4111	37	-13	2	C
ATOM 15643	CD	GLN D 126	86.129	26.544	30.046	1.00	37.36		C
ANISOU15643	CD	GLN D 126	4703	4739	4754	-148	34	45	C
ATOM 15644	OE1	GLN D 126	84.983	26.961	29.862	1.00	40.15		O
ANISOU15644	OE1	GLN D 126	4981	5167	5106	46	21	11	O
ATOM 15645	NE2	GLN D 126	86.397	25.401	30.672	1.00	40.01		N
ANISOU15645	NE2	GLN D 126	5177	4898	5128	1	-84	51	N
ATOM 15751	CA	PHE D 134	84.632	42.192	35.832	1.00	10.46		C
ANISOU15751	CA	PHE D 134	1302	1432	1238	-74	-62	-15	C
ATOM 15753	CB	PHE D 134	84.703	41.176	36.950	1.00	12.21		C
ANISOU15753	CB	PHE D 134	1581	1540	1517	-90	-59	-5	C
ATOM 15756	CG	PHE D 134	85.106	39.837	36.463	1.00	15.32		C
ANISOU15756	CG	PHE D 134	2059	1864	1896	33	144	-71	C
ATOM 15757	CD1	PHE D 134	86.455	39.513	36.347	1.00	18.75		C
ANISOU15757	CD1	PHE D 134	2272	2262	2590	33	-190	-101	C
ATOM 15759	CE1	PHE D 134	86.860	38.325	35.794	1.00	19.22		C
ANISOU15759	CE1	PHE D 134	2492	2280	2528	146	-66	79	C
ATOM 15761	CZ	PHE D 134	85.917	37.427	35.365	1.00	19.54		C
ANISOU15761	CZ	PHE D 134	2609	2161	2653	95	-224	54	C
ATOM 15763	CE2	PHE D 134	84.563	37.730	35.447	1.00	20.85		C
ANISOU15763	CE2	PHE D 134	2773	2374	2774	53	102	-29	C
ATOM 15765	CD2	PHE D 134	84.152	38.976	35.970	1.00	17.98		C
ANISOU15765	CD2	PHE D 134	2496	2122	2213	-103	-4	-28	C
ATOM 15783	CB	TYR D 136	81.679	44.948	41.151	1.00	8.24		C
ANISOU15783	CB	TYR D 136	972	1011	1145	-148	4	96	C
ATOM 15786	CG	TYR D 136	81.061	44.511	42.473	1.00	8.30		C

ANISOU15786	CG	TYR	D	136	1131	1014	1010	213	-280	234	C
ATOM 15787	CD1	TYR	D	136	80.516	43.218	42.622	1.00	9.08		C
ANISOU15787	CD1	TYR	D	136	1072	1289	1087	2	-199	0	C
ATOM 15789	CE1	TYR	D	136	80.073	42.765	43.807	1.00	9.63		C
ANISOU15789	CE1	TYR	D	136	1350	832	1476	-34	117	30	C
ATOM 15791	CZ	TYR	D	136	80.246	43.509	44.958	1.00	8.94		C
ANISOU15791	CZ	TYR	D	136	855	1312	1229	-1	-189	-40	C
ATOM 15792	OH	TYR	D	136	79.775	43.024	46.166	1.00	10.79		O
ANISOU15792	OH	TYR	D	136	1283	1624	1192	-290	-118	-60	O
ATOM 15794	CE2	TYR	D	136	80.743	44.789	44.861	1.00	7.43		C
ANISOU15794	CE2	TYR	D	136	445	1162	1213	-17	-112	176	C
ATOM 15796	CD2	TYR	D	136	81.189	45.268	43.585	1.00	10.13		C
ANISOU15796	CD2	TYR	D	136	1160	1424	1263	235	-192	42	C
ATOM 16347	CA	THR	D	172	87.664	44.843	40.016	1.00	9.27		C
ANISOU16347	CA	THR	D	172	1033	1306	1182	23	41	53	C
ATOM 16349	CB	THR	D	172	86.843	43.644	40.524	1.00	9.86		C
ANISOU16349	CB	THR	D	172	1056	1379	1309	12	-64	55	C
ATOM 16351	OG1	THR	D	172	87.059	42.487	39.688	1.00	11.86		O
ANISOU16351	OG1	THR	D	172	1330	1721	1453	-46	-276	-11	O
ATOM 16353	CG2	THR	D	172	85.341	43.951	40.514	1.00	11.33		C
ANISOU16353	CG2	THR	D	172	1429	1446	1430	61	33	126	C
ATOM 16359	N	GLY	D	173	89.820	43.979	40.764	1.00	10.37		N
ANISOU16359	N	GLY	D	173	1208	1466	1263	20	98	90	N
ATOM 16364	C	GLY	D	173	91.468	42.150	40.212	1.00	11.90		C
ANISOU16364	C	GLY	D	173	1514	1540	1465	20	-43	62	C
ATOM 16365	O	GLY	D	173	92.252	41.407	40.840	1.00	11.81		O
ANISOU16365	O	GLY	D	173	1118	1789	1580	161	-105	47	O
ATOM 16366	N	LEU	D	174	90.825	41.753	39.114	1.00	11.48		N
ANISOU16366	N	LEU	D	174	1474	1519	1367	11	-91	62	N
ATOM 16368	CA	LEU	D	174	90.932	40.406	38.574	1.00	11.20		C
ANISOU16368	CA	LEU	D	174	1451	1499	1303	20	-53	84	C
ATOM 16370	CB	LEU	D	174	89.774	39.510	39.097	1.00	11.10		C
ANISOU16370	CB	LEU	D	174	1256	1622	1339	-1	-100	65	C
ATOM 16373	CG	LEU	D	174	89.745	38.053	38.599	1.00	13.12		C
ANISOU16373	CG	LEU	D	174	1510	1753	1719	44	-82	19	C
ATOM 16375	CD1	LEU	D	174	91.043	37.248	38.882	1.00	12.18		C
ANISOU16375	CD1	LEU	D	174	1541	1289	1798	-34	-155	183	C
ATOM 16379	CD2	LEU	D	174	88.542	37.297	39.098	1.00	16.16		C
ANISOU16379	CD2	LEU	D	174	2140	2104	1895	-105	6	98	C
ATOM 16383	C	LEU	D	174	90.827	40.541	37.063	1.00	11.00		C
ANISOU16383	C	LEU	D	174	1396	1438	1343	1	-25	29	C
ATOM 16384	O	LEU	D	174	89.816	40.980	36.543	1.00	11.81		O
ANISOU16384	O	LEU	D	174	1654	1572	1261	279	-121	120	O
ATOM 16414	CD1	PHE	D	176	89.923	36.340	34.282	1.00	14.36		C
ANISOU16414	CD1	PHE	D	176	1963	1550	1942	-4	159	43	C
ATOM 16416	CE1	PHE	D	176	89.597	35.620	35.407	1.00	15.28		C
ANISOU16416	CE1	PHE	D	176	2005	1945	1856	4	212	50	C
ATOM 16418	CZ	PHE	D	176	90.003	34.310	35.547	1.00	14.97		C
ANISOU16418	CZ	PHE	D	176	2044	1834	1806	31	36	22	C
ATOM 16420	CE2	PHE	D	176	90.774	33.736	34.575	1.00	14.53		C
ANISOU16420	CE2	PHE	D	176	1964	1669	1885	-40	56	45	C
ATOM 16422	CD2	PHE	D	176	91.085	34.447	33.430	1.00	14.76		C
ANISOU16422	CD2	PHE	D	176	1882	1807	1915	33	127	72	C
ATOM 17024	CB	GLU	D	214	81.723	39.400	32.952	1.00	14.76		C
ANISOU17024	CB	GLU	D	214	1869	1902	1836	-44	16	-18	C
ATOM 17052	C	ILE	D	215	79.104	41.058	36.376	1.00	10.12		C
ANISOU17052	C	ILE	D	215	1160	1349	1335	13	28	-32	C
ATOM 17053	O	ILE	D	215	78.620	39.950	36.186	1.00	9.90		O
ANISOU17053	O	ILE	D	215	1504	1284	973	36	-49	106	O
ATOM 17054	N	MET	D	216	79.746	41.388	37.476	1.00	10.21		N
ANISOU17054	N	MET	D	216	1240	1370	1268	-114	92	-14	N

ATOM 17056	CA	MET	D	216	79.795	40.580	38.655	1.00	10.97		C
ANISOU17056	CA	MET	D	216	1346	1380	1439	-6	28	-32	C
ATOM 17058	CB	MET	D	216	81.086	40.796	39.385	1.00	13.21		C
ANISOU17058	CB	MET	D	216	1749	1672	1597	-31	-47	63	C
ATOM 17061	CG	MET	D	216	81.160	40.075	40.718	1.00	12.50		C
ANISOU17061	CG	MET	D	216	1638	1609	1499	-60	-44	183	C
ATOM 17064	SD	MET	D	216	82.853	40.115	41.404	1.00	13.17		S
ANISOU17064	SD	MET	D	216	1370	1819	1812	52	-52	-33	S
ATOM 17065	CE	MET	D	216	83.686	39.307	40.308	1.00	17.09		C
ANISOU17065	CE	MET	D	216	2091	2339	2064	141	74	133	C
ATOM 17069	C	MET	D	216	78.586	41.086	39.502	1.00	10.53		C
ANISOU17069	C	MET	D	216	1298	1433	1270	-10	84	-10	C
ATOM 17070	O	MET	D	216	78.595	42.174	40.074	1.00	9.66		O
ANISOU17070	O	MET	D	216	1067	1237	1365	122	355	68	O
ATOM 17071	N	GLY	D	217	77.583	40.262	39.596	1.00	10.64		N
ANISOU17071	N	GLY	D	217	1407	1293	1340	0	21	-52	N
ATOM 17073	CA	GLY	D	217	76.286	40.650	40.186	1.00	10.02		C
ANISOU17073	CA	GLY	D	217	1220	1356	1229	-33	72	-22	C
ATOM 17076	C	GLY	D	217	76.370	41.005	41.664	1.00	10.26		C
ANISOU17076	C	GLY	D	217	1235	1432	1229	-16	62	-24	C
ATOM 17077	O	GLY	D	217	77.307	40.574	42.368	1.00	10.90		O
ANISOU17077	O	GLY	D	217	1320	1524	1296	18	103	61	O
ATOM 17078	N	ARG	D	218	75.343	41.714	42.152	1.00	9.62		N
ANISOU17078	N	ARG	D	218	1213	1268	1174	-21	-38	-41	N
ATOM 17080	CA	ARG	D	218	75.300	42.189	43.549	1.00	9.84		C
ANISOU17080	CA	ARG	D	218	1181	1311	1246	13	64	14	C
ATOM 17082	CB	ARG	D	218	74.132	43.117	43.724	1.00	9.14		C
ANISOU17082	CB	ARG	D	218	1199	1125	1146	39	-100	-40	C
ATOM 17100	C	ARG	D	218	75.224	41.035	44.556	1.00	9.42		C
ANISOU17100	C	ARG	D	218	1056	1260	1263	92	55	13	C
ATOM 17101	O	ARG	D	218	75.447	41.229	45.716	1.00	9.80		O
ANISOU17101	O	ARG	D	218	1126	1287	1310	145	339	10	O
ATOM 17102	N	GLY	D	219	74.945	39.834	44.101	1.00	9.41		N
ANISOU17102	N	GLY	D	219	1153	1170	1251	3	39	29	N
ATOM 17104	CA	GLY	D	219	74.975	38.662	44.992	1.00	10.78		C
ANISOU17104	CA	GLY	D	219	1468	1355	1272	42	-14	-73	C
ATOM 17107	C	GLY	D	219	76.372	38.214	45.383	1.00	9.62		C
ANISOU17107	C	GLY	D	219	1353	1146	1156	-22	-20	-81	C
ATOM 17108	O	GLY	D	219	76.538	37.469	46.358	1.00	12.23		O
ANISOU17108	O	GLY	D	219	1585	1700	1362	208	-10	51	O
ATOM 17109	N	TYR	D	220	77.387	38.650	44.638	1.00	8.50		N
ANISOU17109	N	TYR	D	220	1233	1130	866	45	-5	-67	N
ATOM 17111	CA	TYR	D	220	78.741	38.381	45.035	1.00	8.93		C
ANISOU17111	CA	TYR	D	220	1326	1044	1021	2	15	71	C
ATOM 17113	CB	TYR	D	220	79.672	38.417	43.883	1.00	9.30		C
ANISOU17113	CB	TYR	D	220	1095	1127	1310	121	-63	62	C
ATOM 17116	CG	TYR	D	220	79.559	37.289	42.919	1.00	9.55		C
ANISOU17116	CG	TYR	D	220	1183	1259	1183	-134	-54	-50	C
ATOM 17117	CD1	TYR	D	220	78.944	37.495	41.697	1.00	11.63		C
ANISOU17117	CD1	TYR	D	220	1295	1705	1417	-33	55	3	C
ATOM 17119	CE1	TYR	D	220	78.840	36.486	40.773	1.00	10.42		C
ANISOU17119	CE1	TYR	D	220	1055	1605	1298	-212	238	-68	C
ATOM 17121	CZ	TYR	D	220	79.343	35.236	41.043	1.00	13.68		C
ANISOU17121	CZ	TYR	D	220	1589	1915	1694	-31	119	6	C
ATOM 17122	OH	TYR	D	220	79.173	34.260	40.070	1.00	16.65		O
ANISOU17122	OH	TYR	D	220	1989	2444	1892	219	163	-247	O
ATOM 17124	CE2	TYR	D	220	79.969	34.959	42.259	1.00	12.72		C
ANISOU17124	CE2	TYR	D	220	1457	1554	1819	124	-87	-19	C
ATOM 17126	CD2	TYR	D	220	80.063	36.010	43.210	1.00	14.00		C
ANISOU17126	CD2	TYR	D	220	1639	1879	1798	173	-258	-125	C
ATOM 17128	C	TYR	D	220	79.219	39.460	45.974	1.00	9.29		C

ANISOU17128	C	TYR	D	220	1285	1200	1043	-60	-8	40	C
ATOM 17129	O	TYR	D	220	78.739	40.599	45.932	1.00	8.95		O
ANISOU17129	O	TYR	D	220	1486	1208	706	-47	25	147	O
ATOM 17130	N	ALA	D	221	80.171	39.097	46.809	1.00	10.54		N
ANISOU17130	N	ALA	D	221	1430	1350	1222	29	-12	115	N
ATOM 17132	CA	ALA	D	221	80.915	40.100	47.591	1.00	11.67		C
ANISOU17132	CA	ALA	D	221	1519	1485	1427	-1	33	58	C
ATOM 17134	CB	ALA	D	221	81.208	39.639	49.036	1.00	13.33		C
ANISOU17134	CB	ALA	D	221	1815	1689	1558	90	30	59	C
ATOM 17138	C	ALA	D	221	82.248	40.316	46.928	1.00	11.26		C
ANISOU17138	C	ALA	D	221	1445	1525	1306	-17	16	92	C
ATOM 17139	O	ALA	D	221	82.997	39.363	46.707	1.00	10.50		O
ANISOU17139	O	ALA	D	221	1450	1341	1196	-233	293	116	O
ATOM 17140	N	TRP	D	222	82.573	41.572	46.761	1.00	10.18		N
ANISOU17140	N	TRP	D	222	1286	1393	1188	-80	16	48	N
ATOM 17142	CA	TRP	D	222	83.880	42.007	46.261	1.00	10.95		C
ANISOU17142	CA	TRP	D	222	1199	1593	1368	1	11	56	C
ATOM 17144	CB	TRP	D	222	83.875	42.542	44.843	1.00	11.21		C
ANISOU17144	CB	TRP	D	222	1257	1591	1410	-39	-13	68	C
ATOM 17147	CG	TRP	D	222	85.231	43.127	44.491	1.00	10.60		C
ANISOU17147	CG	TRP	D	222	1238	1599	1189	-6	62	79	C
ATOM 17148	CD1	TRP	D	222	86.424	42.471	44.575	1.00	13.24		C
ANISOU17148	CD1	TRP	D	222	1526	1769	1735	30	40	17	C
ATOM 17150	NE1	TRP	D	222	87.447	43.319	44.232	1.00	12.16		N
ANISOU17150	NE1	TRP	D	222	1387	1898	1333	118	211	4	N
ATOM 17152	CE2	TRP	D	222	86.944	44.552	43.936	1.00	12.39		C
ANISOU17152	CE2	TRP	D	222	1608	1662	1436	13	200	101	C
ATOM 17153	CD2	TRP	D	222	85.554	44.486	44.115	1.00	10.71		C
ANISOU17153	CD2	TRP	D	222	1416	1567	1084	21	-79	12	C
ATOM 17154	CE3	TRP	D	222	84.801	45.624	43.825	1.00	12.02		C
ANISOU17154	CE3	TRP	D	222	1432	1652	1483	-23	222	37	C
ATOM 17160	CZ2	TRP	D	222	87.598	45.723	43.521	1.00	13.11		C
ANISOU17160	CZ2	TRP	D	222	1718	1601	1660	-57	112	-87	C
ATOM 17162	C	TRP	D	222	84.333	43.101	47.219	1.00	11.40		C
ANISOU17162	C	TRP	D	222	1389	1494	1446	-19	129	47	C
ATOM 17163	O	TRP	D	222	83.747	44.182	47.270	1.00	11.18		O
ANISOU17163	O	TRP	D	222	1153	1578	1514	-53	84	69	O
ATOM 17164	N	LEU	D	223	85.317	42.761	48.039	1.00	10.67		N
ANISOU17164	N	LEU	D	223	986	1485	1580	151	142	-28	N
ATOM 17166	CA	LEU	D	223	85.830	43.596	49.104	1.00	13.05		C
ANISOU17166	CA	LEU	D	223	1548	1692	1715	77	71	3	C
ATOM 17168	CB	LEU	D	223	85.705	42.886	50.389	1.00	13.78		C
ANISOU17168	CB	LEU	D	223	1628	1836	1770	36	87	-50	C
ATOM 17171	CG	LEU	D	223	84.283	42.494	50.695	1.00	14.22		C
ANISOU17171	CG	LEU	D	223	1729	1930	1742	-16	36	-38	C
ATOM 17173	CD1	LEU	D	223	84.200	41.818	52.105	1.00	16.38		C
ANISOU17173	CD1	LEU	D	223	2112	2206	1905	44	106	1	C
ATOM 17177	CD2	LEU	D	223	83.374	43.699	50.564	1.00	14.71		C
ANISOU17177	CD2	LEU	D	223	1834	2014	1738	-12	180	181	C
ATOM 17181	C	LEU	D	223	87.289	43.948	48.867	1.00	14.62		C
ANISOU17181	C	LEU	D	223	1719	1967	1868	24	36	59	C
ATOM 17182	O	LEU	D	223	88.004	43.175	48.239	1.00	15.86		O
ANISOU17182	O	LEU	D	223	1776	2100	2149	75	103	168	O
ATOM 17183	N	ASP	D	224	87.682	45.129	49.312	1.00	17.34		N
ANISOU17183	N	ASP	D	224	2155	2372	2061	-7	7	-20	N
ATOM 17185	CA	ASP	D	224	89.039	45.680	49.123	1.00	19.46		C
ANISOU17185	CA	ASP	D	224	2428	2613	2351	-7	-59	-90	C
ATOM 17203	CG2	THR	D	225	90.714	42.756	52.661	1.00	19.72		C
ANISOU17203	CG2	THR	D	225	2592	2607	2294	90	124	-5	C
ATOM 17323	O	GLU	D	233	83.967	42.453	57.169	1.00	10.64		O
ANISOU17323	O	GLU	D	233	1370	1402	1270	6	-41	125	O

ATOM 17324	N	ALA D 234	85.971	43.140	56.424	1.00	9.92		N
ANISOU17324	N	ALA D 234	1185	1258	1324	-50	18	1	N
ATOM 17326	CA	ALA D 234	86.198	41.869	55.728	1.00	9.91		C
ANISOU17326	CA	ALA D 234	1161	1305	1297	-33	-18	35	C
ATOM 17328	CB	ALA D 234	87.337	41.987	54.747	1.00	9.20		C
ANISOU17328	CB	ALA D 234	994	1309	1189	83	-61	37	C
ATOM 17332	C	ALA D 234	86.387	40.721	56.727	1.00	9.56		C
ANISOU17332	C	ALA D 234	1182	1184	1264	-25	16	-20	C
ATOM 17333	O	ALA D 234	85.864	39.641	56.501	1.00	9.49		O
ANISOU17333	O	ALA D 234	1211	1138	1257	-159	134	-57	O
ATOM 17334	N	GLY D 235	87.099	40.963	57.837	1.00	9.32		N
ANISOU17334	N	GLY D 235	1217	1055	1267	39	40	-38	N
ATOM 17336	CA	GLY D 235	87.228	39.971	58.862	1.00	9.85		C
ANISOU17336	CA	GLY D 235	1234	1316	1190	-62	-8	14	C
ATOM 17339	C	GLY D 235	85.894	39.550	59.457	1.00	9.55		C
ANISOU17339	C	GLY D 235	1104	1274	1247	3	-20	66	C
ATOM 17340	O	GLY D 235	85.631	38.347	59.656	1.00	9.98		O
ANISOU17340	O	GLY D 235	1023	1375	1392	-252	200	106	O
ATOM 17356	C	GLN D 236	82.969	39.394	59.233	1.00	9.90		C
ANISOU17356	C	GLN D 236	1364	1174	1223	30	-2	-8	C
ATOM 17357	O	GLN D 236	82.249	38.525	59.581	1.00	9.00		O
ANISOU17357	O	GLN D 236	1476	1127	814	-56	-162	172	O
ATOM 17358	N	PHE D 237	83.110	39.750	57.961	1.00	10.41		N
ANISOU17358	N	PHE D 237	1459	1407	1088	-78	-51	36	N
ATOM 17360	CA	PHE D 237	82.326	39.101	56.888	1.00	11.16		C
ANISOU17360	CA	PHE D 237	1485	1377	1378	-97	-9	7	C
ATOM 17362	CB	PHE D 237	82.584	39.817	55.570	1.00	13.02		C
ANISOU17362	CB	PHE D 237	1822	1596	1527	-99	-12	20	C
ATOM 17365	CG	PHE D 237	81.695	39.367	54.431	1.00	13.04		C
ANISOU17365	CG	PHE D 237	1842	1672	1440	-104	-91	214	C
ATOM 17366	CD1	PHE D 237	80.375	39.840	54.326	1.00	17.86		C
ANISOU17366	CD1	PHE D 237	2230	2389	2165	-187	-160	31	C
ATOM 17368	CE1	PHE D 237	79.570	39.443	53.278	1.00	17.98		C
ANISOU17368	CE1	PHE D 237	2216	2415	2199	-82	-69	19	C
ATOM 17370	CZ	PHE D 237	80.020	38.522	52.415	1.00	17.15		C
ANISOU17370	CZ	PHE D 237	2274	2347	1894	-105	-96	-102	C
ATOM 17372	CE2	PHE D 237	81.270	38.067	52.466	1.00	18.28		C
ANISOU17372	CE2	PHE D 237	2500	2291	2154	-39	-299	177	C
ATOM 17374	CD2	PHE D 237	82.157	38.508	53.512	1.00	17.71		C
ANISOU17374	CD2	PHE D 237	2752	1883	2094	-193	-189	94	C
ATOM 17376	C	PHE D 237	82.683	37.610	56.852	1.00	11.00		C
ANISOU17376	C	PHE D 237	1429	1445	1303	-23	-18	27	C
ATOM 17377	O	PHE D 237	81.792	36.740	56.926	1.00	11.74		O
ANISOU17377	O	PHE D 237	1499	1388	1571	-62	-136	36	O
ATOM 17378	N	ILE D 238	83.978	37.322	56.768	1.00	10.34		N
ANISOU17378	N	ILE D 238	1224	1297	1407	7	-20	3	N
ATOM 17380	CA	ILE D 238	84.496	35.934	56.802	1.00	9.68		C
ANISOU17380	CA	ILE D 238	1177	1232	1269	-61	-74	-40	C
ATOM 17382	CB	ILE D 238	86.050	35.926	56.566	1.00	9.49		C
ANISOU17382	CB	ILE D 238	1260	1190	1156	19	33	10	C
ATOM 17384	CG1	ILE D 238	86.370	36.507	55.187	1.00	9.12		C
ANISOU17384	CG1	ILE D 238	1246	1063	1153	16	8	-127	C
ATOM 17387	CD1	ILE D 238	85.738	35.752	54.097	1.00	10.39		C
ANISOU17387	CD1	ILE D 238	1148	1487	1313	-394	11	44	C
ATOM 17391	CG2	ILE D 238	86.578	34.517	56.744	1.00	10.22		C
ANISOU17391	CG2	ILE D 238	1080	1424	1378	135	-1	-138	C
ATOM 17395	C	ILE D 238	84.124	35.193	58.062	1.00	9.64		C
ANISOU17395	C	ILE D 238	1158	1238	1264	17	44	-108	C
ATOM 17396	O	ILE D 238	83.667	34.023	58.023	1.00	10.60		O
ANISOU17396	O	ILE D 238	1635	1086	1306	-6	203	-209	O
ATOM 17397	N	ALA D 239	84.230	35.860	59.205	1.00	8.72		N

ANISOU17397	N	ALA D 239	1119	1073	1120	-90	-265	-66	N
ATOM 17399	CA	ALA D 239	83.832	35.199	60.434	1.00	8.91		C
ANISOU17399	CA	ALA D 239	972	1190	1222	26	6	-75	C
ATOM 17401	CB	ALA D 239	84.145	36.075	61.650	1.00	9.70		C
ANISOU17401	CB	ALA D 239	1055	1285	1346	-41	-117	-82	C
ATOM 17405	C	ALA D 239	82.392	34.765	60.461	1.00	8.94		C
ANISOU17405	C	ALA D 239	1137	1099	1161	-69	-7	-101	C
ATOM 17406	O	ALA D 239	82.072	33.664	60.912	1.00	10.83		O
ANISOU17406	O	ALA D 239	1489	1328	1297	-16	116	-148	O
ATOM 17407	N	THR D 240	81.529	35.637	60.018	1.00	7.67		N
ANISOU17407	N	THR D 240	908	984	1021	-119	-19	-7	N
ATOM 17409	CA	THR D 240	80.127	35.326	60.030	1.00	9.37		C
ANISOU17409	CA	THR D 240	1124	1086	1349	-13	-116	-113	C
ATOM 17411	CB	THR D 240	79.340	36.571	59.619	1.00	9.96		C
ANISOU17411	CB	THR D 240	1150	1162	1471	-8	28	-82	C
ATOM 17415	CG2	THR D 240	77.837	36.220	59.476	1.00	9.38		C
ANISOU17415	CG2	THR D 240	1144	932	1488	172	-102	-18	C
ATOM 17419	C	THR D 240	79.840	34.084	59.138	1.00	8.95		C
ANISOU17419	C	THR D 240	1091	1103	1203	-2	-153	-99	C
ATOM 17420	O	THR D 240	79.115	33.191	59.546	1.00	9.27		O
ANISOU17420	O	THR D 240	1167	1036	1319	-98	-359	-259	O
ATOM 17421	N	LEU D 241	80.409	34.038	57.960	1.00	8.78		N
ANISOU17421	N	LEU D 241	891	1102	1343	8	-170	-128	N
ATOM 17423	CA	LEU D 241	80.168	32.879	57.093	1.00	10.06		C
ANISOU17423	CA	LEU D 241	1243	1256	1324	46	-64	-95	C
ATOM 17425	CB	LEU D 241	80.808	33.119	55.742	1.00	9.33		C
ANISOU17425	CB	LEU D 241	1023	1197	1325	-116	9	-68	C
ATOM 17428	CG	LEU D 241	80.149	34.154	54.845	1.00	13.37		C
ANISOU17428	CG	LEU D 241	1648	1483	1946	-79	-28	-64	C
ATOM 17430	CD1	LEU D 241	81.022	34.419	53.697	1.00	17.22		C
ANISOU17430	CD1	LEU D 241	2408	2044	2088	24	1	40	C
ATOM 17434	CD2	LEU D 241	78.751	33.692	54.349	1.00	15.10		C
ANISOU17434	CD2	LEU D 241	1673	1912	2152	254	-336	11	C
ATOM 17438	C	LEU D 241	80.742	31.608	57.697	1.00	8.96		C
ANISOU17438	C	LEU D 241	1113	1115	1173	33	4	-107	C
ATOM 17439	O	LEU D 241	80.102	30.557	57.718	1.00	8.90		O
ANISOU17439	O	LEU D 241	963	1262	1156	-52	173	-69	O
ATOM 17440	N	GLU D 242	81.995	31.679	58.147	1.00	9.68		N
ANISOU17440	N	GLU D 242	1138	1142	1397	-101	1	-71	N
ATOM 17442	CA	GLU D 242	82.670	30.480	58.686	1.00	9.14		C
ANISOU17442	CA	GLU D 242	1147	1113	1210	-46	-33	-53	C
ATOM 17444	CB	GLU D 242	84.155	30.731	58.948	1.00	9.67		C
ANISOU17444	CB	GLU D 242	1203	1145	1324	-63	31	-74	C
ATOM 17447	CG	GLU D 242	84.904	31.076	57.692	1.00	9.65		C
ANISOU17447	CG	GLU D 242	1367	1208	1089	-97	-6	-44	C
ATOM 17450	CD	GLU D 242	86.413	31.074	57.882	1.00	10.27		C
ANISOU17450	CD	GLU D 242	1282	1385	1234	77	-32	69	C
ATOM 17451	OE1	GLU D 242	86.862	31.189	59.054	1.00	11.33		O
ANISOU17451	OE1	GLU D 242	1610	1426	1268	-24	-42	174	O
ATOM 17452	OE2	GLU D 242	87.153	31.009	56.876	1.00	10.26		O
ANISOU17452	OE2	GLU D 242	1603	1242	1053	50	-24	207	O
ATOM 17453	C	GLU D 242	82.000	29.908	59.931	1.00	10.23		C
ANISOU17453	C	GLU D 242	1289	1279	1319	-7	-9	-35	C
ATOM 17454	O	GLU D 242	81.831	28.680	60.073	1.00	11.36		O
ANISOU17454	O	GLU D 242	1594	1323	1396	-184	151	-96	O
ATOM 17455	N	ASN D 243	81.602	30.796	60.826	1.00	10.17		N
ANISOU17455	N	ASN D 243	1302	1250	1312	-103	0	-73	N
ATOM 17457	CA	ASN D 243	80.889	30.381	62.011	1.00	10.80		C
ANISOU17457	CA	ASN D 243	1447	1390	1266	-7	-4	15	C
ATOM 17459	CB	ASN D 243	81.067	31.483	63.074	1.00	11.99		C
ANISOU17459	CB	ASN D 243	1663	1426	1465	-69	105	25	C

ANISOU17530	CD2	LEU	D	247	1268	1257	1299	89	23	42	C
ATOM 17534	C	LEU	D	247	84.162	26.866	56.366	1.00	11.86		C
ANISOU17534	C	LEU	D	247	1403	1410	1693	28	28	-63	C
ATOM 17535	O	LEU	D	247	83.704	27.938	56.752	1.00	14.02		O
ANISOU17535	O	LEU	D	247	1588	1546	2192	-194	104	-299	O
ATOM 17536	N	LYS	D	248	85.383	26.756	55.875	1.00	10.39		N
ANISOU17536	N	LYS	D	248	1145	1359	1441	44	-85	-85	N
ATOM 17538	CA	LYS	D	248	86.263	27.878	55.871	1.00	12.66		C
ANISOU17538	CA	LYS	D	248	1579	1509	1721	65	-19	-22	C
ATOM 17540	CB	LYS	D	248	87.644	27.460	56.411	1.00	13.65		C
ANISOU17540	CB	LYS	D	248	1494	1711	1980	-92	-155	-3	C
ATOM 17543	CG	LYS	D	248	87.523	27.217	57.955	1.00	18.20		C
ANISOU17543	CG	LYS	D	248	2272	2371	2270	25	26	82	C
ATOM 17546	CD	LYS	D	248	88.857	27.304	58.829	1.00	23.61		C
ANISOU17546	CD	LYS	D	248	2890	2952	3128	-46	-130	-7	C
ATOM 17549	CE	LYS	D	248	88.575	27.730	60.314	1.00	25.17		C
ANISOU17549	CE	LYS	D	248	3229	3182	3153	-114	28	59	C
ATOM 17552	NZ	LYS	D	248	87.112	27.569	60.916	1.00	26.16		N
ANISOU17552	NZ	LYS	D	248	3057	3409	3474	-121	-34	-90	N
ATOM 17556	C	LYS	D	248	86.377	28.438	54.484	1.00	12.32		C
ANISOU17556	C	LYS	D	248	1527	1557	1597	14	-26	-63	C
ATOM 17557	O	LYS	D	248	86.264	27.696	53.563	1.00	13.54		O
ANISOU17557	O	LYS	D	248	1686	1664	1794	-15	-6	-151	O
ATOM 17558	N	VAL	D	249	86.521	29.759	54.356	1.00	12.28		N
ANISOU17558	N	VAL	D	249	1533	1537	1595	13	21	27	N
ATOM 17560	CA	VAL	D	249	86.761	30.428	53.063	1.00	10.47		C
ANISOU17560	CA	VAL	D	249	1310	1340	1327	74	-30	-56	C
ATOM 17562	CB	VAL	D	249	86.245	31.836	53.126	1.00	10.52		C
ANISOU17562	CB	VAL	D	249	1205	1421	1369	-40	-15	12	C
ATOM 17564	CG1	VAL	D	249	86.497	32.608	51.811	1.00	9.89		C
ANISOU17564	CG1	VAL	D	249	1284	1252	1221	112	-177	-129	C
ATOM 17568	CG2	VAL	D	249	84.696	31.786	53.566	1.00	12.00		C
ANISOU17568	CG2	VAL	D	249	1357	1636	1567	211	-84	-167	C
ATOM 17572	C	VAL	D	249	88.263	30.487	52.746	1.00	9.56		C
ANISOU17572	C	VAL	D	249	1199	1149	1283	3	-57	40	C
ATOM 17573	O	VAL	D	249	89.079	30.898	53.593	1.00	11.33		O
ANISOU17573	O	VAL	D	249	1655	1212	1437	237	14	67	O
ATOM 17574	N	ALA	D	250	88.623	30.110	51.521	1.00	8.67		N
ANISOU17574	N	ALA	D	250	930	1076	1286	66	-51	-10	N
ATOM 17576	CA	ALA	D	250	89.982	30.297	50.984	1.00	9.78		C
ANISOU17576	CA	ALA	D	250	1258	1222	1233	-55	-33	5	C
ATOM 17578	CB	ALA	D	250	90.320	31.801	50.906	1.00	10.37		C
ANISOU17578	CB	ALA	D	250	1321	1308	1310	-74	-55	-53	C
ATOM 17582	C	ALA	D	250	91.034	29.523	51.719	1.00	10.82		C
ANISOU17582	C	ALA	D	250	1253	1360	1497	-27	-12	-16	C
ATOM 17583	O	ALA	D	250	92.144	30.025	51.970	1.00	11.65		O
ANISOU17583	O	ALA	D	250	1494	1365	1565	-62	-214	-214	O
ATOM 17584	N	CYS	D	251	90.677	28.282	52.068	1.00	10.30		N
ANISOU17584	N	CYS	D	251	1154	1303	1455	-49	-42	18	N
ATOM 17586	CA	CYS	D	251	91.629	27.335	52.576	1.00	12.13		C
ANISOU17586	CA	CYS	D	251	1544	1517	1548	14	66	-30	C
ATOM 17588	CB	CYS	D	251	90.869	26.351	53.463	1.00	13.20		C
ANISOU17588	CB	CYS	D	251	1639	1499	1876	-121	-126	4	C
ATOM 17591	SG	CYS	D	251	91.783	24.962	54.066	1.00	16.67		S
ANISOU17591	SG	CYS	D	251	2349	1960	2024	345	192	-257	S
ATOM 17592	C	CYS	D	251	92.276	26.697	51.334	1.00	11.58		C
ANISOU17592	C	CYS	D	251	1378	1478	1541	73	-31	5	C
ATOM 17593	O	CYS	D	251	91.712	25.835	50.692	1.00	10.00		O
ANISOU17593	O	CYS	D	251	949	1384	1466	230	-178	-85	O
ATOM 17594	N	PRO	D	252	93.517	27.041	51.040	1.00	12.29		N
ANISOU17594	N	PRO	D	252	1595	1509	1564	-1	6	41	N

ATOM 17595	CA	PRO D 252	94.151	26.454	49.872	1.00	12.63		C
ANISOU17595	CA	PRO D 252	1599	1547	1652	24	23	-27	C
ATOM 17597	CB	PRO D 252	95.561	27.090	49.877	1.00	13.83		C
ANISOU17597	CB	PRO D 252	1695	1806	1752	43	-13	-68	C
ATOM 17600	CG	PRO D 252	95.455	28.314	50.664	1.00	13.60		C
ANISOU17600	CG	PRO D 252	1818	1682	1667	-32	-55	42	C
ATOM 17603	CD	PRO D 252	94.416	27.987	51.712	1.00	12.32		C
ANISOU17603	CD	PRO D 252	1449	1608	1622	118	33	-18	C
ATOM 17606	C	PRO D 252	94.262	24.907	49.917	1.00	12.73		C
ANISOU17606	C	PRO D 252	1661	1573	1602	-32	-2	-21	C
ATOM 17607	O	PRO D 252	94.139	24.252	48.855	1.00	10.69		O
ANISOU17607	O	PRO D 252	1340	1295	1425	81	30	-149	O
ATOM 17608	N	GLU D 253	94.479	24.359	51.112	1.00	11.57		N
ANISOU17608	N	GLU D 253	1372	1503	1521	6	-23	-12	N
ATOM 17610	CA	GLU D 253	94.599	22.950	51.231	1.00	11.36		C
ANISOU17610	CA	GLU D 253	1396	1443	1475	-9	26	-28	C
ATOM 17612	CB	GLU D 253	94.893	22.524	52.650	1.00	12.35		C
ANISOU17612	CB	GLU D 253	1568	1557	1564	43	25	-77	C
ATOM 17615	CG	GLU D 253	96.232	23.043	53.211	1.00	12.82		C
ANISOU17615	CG	GLU D 253	1513	1739	1619	69	-93	40	C
ATOM 17618	CD	GLU D 253	96.092	24.416	53.851	1.00	15.06		C
ANISOU17618	CD	GLU D 253	1960	1944	1818	-35	45	13	C
ATOM 17619	OE1	GLU D 253	95.088	25.122	53.577	1.00	15.96		O
ANISOU17619	OE1	GLU D 253	1869	2104	2091	-144	182	259	O
ATOM 17620	OE2	GLU D 253	96.962	24.794	54.663	1.00	18.42		O
ANISOU17620	OE2	GLU D 253	2356	2464	2178	-65	-199	199	O
ATOM 17621	C	GLU D 253	93.308	22.310	50.783	1.00	10.72		C
ANISOU17621	C	GLU D 253	1305	1401	1364	1	41	-31	C
ATOM 17622	O	GLU D 253	93.331	21.269	50.156	1.00	9.53		O
ANISOU17622	O	GLU D 253	1127	1246	1246	-16	189	-121	O
ATOM 17623	N	GLU D 254	92.171	22.882	51.169	1.00	10.16		N
ANISOU17623	N	GLU D 254	1339	1180	1339	30	26	-47	N
ATOM 17625	CA	GLU D 254	90.877	22.300	50.818	1.00	10.38		C
ANISOU17625	CA	GLU D 254	1240	1324	1377	28	61	13	C
ATOM 17627	CB	GLU D 254	89.723	23.078	51.490	1.00	10.49		C
ANISOU17627	CB	GLU D 254	1355	1240	1390	54	76	63	C
ATOM 17630	CG	GLU D 254	88.365	22.725	50.928	1.00	9.86		C
ANISOU17630	CG	GLU D 254	1286	1258	1202	32	19	74	C
ATOM 17633	CD	GLU D 254	87.178	23.264	51.732	1.00	10.27		C
ANISOU17633	CD	GLU D 254	1305	1124	1473	113	-35	109	C
ATOM 17634	OE1	GLU D 254	87.308	24.203	52.538	1.00	10.92		O
ANISOU17634	OE1	GLU D 254	1285	1650	1212	263	96	-62	O
ATOM 17635	OE2	GLU D 254	86.107	22.687	51.569	1.00	13.32		O
ANISOU17635	OE2	GLU D 254	1169	1985	1907	136	-129	-213	O
ATOM 17636	C	GLU D 254	90.663	22.354	49.347	1.00	10.66		C
ANISOU17636	C	GLU D 254	1252	1381	1417	65	92	-20	C
ATOM 17637	O	GLU D 254	90.253	21.385	48.703	1.00	10.32		O
ANISOU17637	O	GLU D 254	846	1578	1495	-44	38	83	O
ATOM 17638	N	ILE D 255	90.940	23.518	48.787	1.00	11.98		N
ANISOU17638	N	ILE D 255	1535	1477	1539	47	77	2	N
ATOM 17640	CA	ILE D 255	90.747	23.674	47.347	1.00	13.04		C
ANISOU17640	CA	ILE D 255	1712	1604	1635	22	43	-8	C
ATOM 17642	CB	ILE D 255	90.945	25.118	46.973	1.00	12.67		C
ANISOU17642	CB	ILE D 255	1597	1561	1655	25	71	14	C
ATOM 17644	CG1	ILE D 255	89.826	25.962	47.614	1.00	11.77		C
ANISOU17644	CG1	ILE D 255	1609	1434	1427	33	35	138	C
ATOM 17647	CD1	ILE D 255	90.109	27.449	47.533	1.00	14.33		C
ANISOU17647	CD1	ILE D 255	1918	1525	2000	-52	-21	-123	C
ATOM 17651	CG2	ILE D 255	90.892	25.312	45.454	1.00	14.11		C
ANISOU17651	CG2	ILE D 255	1799	1816	1744	-11	25	-54	C
ATOM 17655	C	ILE D 255	91.630	22.707	46.534	1.00	12.88		C

ANISOU17655	C	ILE	D	255	1635	1627	1632	-4	42	21	C
ATOM 17656	O	ILE	D	255	91.155	22.120	45.522	1.00	13.53		O
ANISOU17656	O	ILE	D	255	1719	1564	1857	-46	139	-49	O
ATOM 17657	N	ALA	D	256	92.886	22.545	46.948	1.00	12.83		N
ANISOU17657	N	ALA	D	256	1707	1541	1627	-75	2	2	N
ATOM 17659	CA	ALA	D	256	93.806	21.660	46.270	1.00	12.69		C
ANISOU17659	CA	ALA	D	256	1620	1559	1643	-67	-16	28	C
ATOM 17661	CB	ALA	D	256	95.186	21.703	46.914	1.00	12.48		C
ANISOU17661	CB	ALA	D	256	1738	1365	1636	-20	-69	23	C
ATOM 17665	C	ALA	D	256	93.238	20.234	46.292	1.00	12.93		C
ANISOU17665	C	ALA	D	256	1687	1534	1689	-37	-17	-14	C
ATOM 17666	O	ALA	D	256	93.288	19.521	45.308	1.00	12.82		O
ANISOU17666	O	ALA	D	256	1507	1743	1619	-50	-120	-83	O
ATOM 17667	N	TYR	D	257	92.679	19.876	47.433	1.00	13.10		N
ANISOU17667	N	TYR	D	257	1667	1647	1664	-5	0	-29	N
ATOM 17669	CA	TYR	D	257	92.116	18.543	47.648	1.00	13.18		C
ANISOU17669	CA	TYR	D	257	1638	1692	1675	15	15	-1	C
ATOM 17671	CB	TYR	D	257	91.736	18.365	49.100	1.00	13.75		C
ANISOU17671	CB	TYR	D	257	1644	1828	1751	104	-75	7	C
ATOM 17674	CG	TYR	D	257	91.174	16.983	49.425	1.00	17.24		C
ANISOU17674	CG	TYR	D	257	2251	2168	2128	-113	-95	24	C
ATOM 17675	CD1	TYR	D	257	91.885	15.831	49.098	1.00	20.81		C
ANISOU17675	CD1	TYR	D	257	2661	2631	2613	-21	-8	-44	C
ATOM 17677	CE1	TYR	D	257	91.401	14.559	49.408	1.00	22.03		C
ANISOU17677	CE1	TYR	D	257	2942	2682	2745	-74	-75	0	C
ATOM 17679	CZ	TYR	D	257	90.184	14.416	50.069	1.00	23.82		C
ANISOU17679	CZ	TYR	D	257	3108	2974	2966	-67	-59	29	C
ATOM 17680	OH	TYR	D	257	89.700	13.137	50.359	1.00	26.01		O
ANISOU17680	OH	TYR	D	257	3521	3142	3219	-315	-26	114	O
ATOM 17682	CE2	TYR	D	257	89.454	15.514	50.412	1.00	23.15		C
ANISOU17682	CE2	TYR	D	257	2982	2924	2888	-96	65	-6	C
ATOM 17684	CD2	TYR	D	257	89.954	16.827	50.087	1.00	22.70		C
ANISOU17684	CD2	TYR	D	257	2871	2974	2778	-141	16	-29	C
ATOM 17686	C	TYR	D	257	90.908	18.337	46.751	1.00	13.24		C
ANISOU17686	C	TYR	D	257	1736	1722	1570	0	-20	33	C
ATOM 17687	O	TYR	D	257	90.816	17.345	46.018	1.00	13.63		O
ANISOU17687	O	TYR	D	257	1677	1955	1545	36	-133	59	O
ATOM 17688	N	ARG	D	258	89.993	19.279	46.798	1.00	14.41		N
ANISOU17688	N	ARG	D	258	1837	1979	1659	29	-31	-101	N
ATOM 17690	CA	ARG	D	258	88.755	19.216	46.003	1.00	16.24		C
ANISOU17690	CA	ARG	D	258	2019	2114	2037	26	-25	-17	C
ATOM 17692	CB	ARG	D	258	87.841	20.389	46.321	1.00	16.33		C
ANISOU17692	CB	ARG	D	258	2007	2111	2085	76	-8	-38	C
ATOM 17695	CG	ARG	D	258	87.223	20.284	47.697	1.00	16.95		C
ANISOU17695	CG	ARG	D	258	2270	2071	2099	-17	21	115	C
ATOM 17698	CD	ARG	D	258	86.167	21.326	48.019	1.00	19.07		C
ANISOU17698	CD	ARG	D	258	2335	2284	2626	-55	10	-44	C
ATOM 17701	NE	ARG	D	258	84.890	21.171	47.296	1.00	21.94		N
ANISOU17701	NE	ARG	D	258	2760	2903	2673	-38	-16	19	N
ATOM 17703	CZ	ARG	D	258	83.883	20.451	47.786	1.00	21.56		C
ANISOU17703	CZ	ARG	D	258	2746	2650	2796	-135	-103	-16	C
ATOM 17704	NH1	ARG	D	258	84.100	19.771	48.937	1.00	21.80		N
ANISOU17704	NH1	ARG	D	258	2764	2946	2573	-256	198	-103	N
ATOM 17707	NH2	ARG	D	258	82.718	20.327	47.128	1.00	19.77		N
ANISOU17707	NH2	ARG	D	258	2533	2291	2687	330	150	104	N
ATOM 17710	C	ARG	D	258	89.061	19.159	44.524	1.00	16.74		C
ANISOU17710	C	ARG	D	258	2120	2191	2048	64	-37	-34	C
ATOM 17711	O	ARG	D	258	88.360	18.475	43.790	1.00	17.91		O
ANISOU17711	O	ARG	D	258	2261	2300	2242	-83	-50	-101	O
ATOM 17712	N	GLN	D	259	90.106	19.853	44.091	1.00	17.73		N
ANISOU17712	N	GLN	D	259	2186	2297	2250	-8	-23	-16	N

ATOM 17714	CA	GLN	D	259	90.532	19.820	42.670	1.00	18.78		C
ANISOU17714	CA	GLN	D	259	2419	2454	2261	35	-56	-14	C
ATOM 17716	CB	GLN	D	259	91.365	21.036	42.348	1.00	19.38		C
ANISOU17716	CB	GLN	D	259	2406	2694	2263	-28	-7	-11	C
ATOM 17719	CG	GLN	D	259	90.705	22.309	42.640	1.00	24.77		C
ANISOU17719	CG	GLN	D	259	3246	3077	3088	23	-49	-92	C
ATOM 17722	CD	GLN	D	259	90.111	22.971	41.425	1.00	29.62		C
ANISOU17722	CD	GLN	D	259	3908	3703	3641	114	-125	88	C
ATOM 17723	OE1	GLN	D	259	89.694	22.307	40.451	1.00	32.16		O
ANISOU17723	OE1	GLN	D	259	4119	4147	3953	-67	-212	-41	O
ATOM 17724	NE2	GLN	D	259	90.059	24.276	41.472	1.00	31.75		N
ANISOU17724	NE2	GLN	D	259	4181	3672	4209	-185	-93	38	N
ATOM 17727	C	GLN	D	259	91.386	18.618	42.311	1.00	18.70		C
ANISOU17727	C	GLN	D	259	2401	2462	2243	11	-37	0	C
ATOM 17728	O	GLN	D	259	91.844	18.478	41.173	1.00	17.88		O
ANISOU17728	O	GLN	D	259	2539	2212	2041	81	-131	-57	O
ATOM 17729	N	LYS	D	260	91.669	17.788	43.309	1.00	18.20		N
ANISOU17729	N	LYS	D	260	2365	2294	2257	9	-21	9	N
ATOM 17731	CA	LYS	D	260	92.471	16.590	43.122	1.00	18.47		C
ANISOU17731	CA	LYS	D	260	2282	2410	2324	-16	3	-7	C
ATOM 17733	CB	LYS	D	260	91.831	15.692	42.021	1.00	18.97		C
ANISOU17733	CB	LYS	D	260	2460	2415	2333	-9	59	-75	C
ATOM 17736	CG	LYS	D	260	90.374	15.337	42.347	1.00	22.40		C
ANISOU17736	CG	LYS	D	260	2735	2935	2840	-6	-17	-18	C
ATOM 17739	CD	LYS	D	260	89.771	14.244	41.455	1.00	27.30		C
ANISOU17739	CD	LYS	D	260	3441	3473	3458	-129	-39	-65	C
ATOM 17742	CE	LYS	D	260	88.360	13.894	41.958	1.00	29.40		C
ANISOU17742	CE	LYS	D	260	3618	3768	3784	-35	32	7	C
ATOM 17745	NZ	LYS	D	260	87.761	15.051	42.698	1.00	31.87		N
ANISOU17745	NZ	LYS	D	260	4090	3979	4040	14	77	-55	N
ATOM 17749	C	LYS	D	260	93.950	16.893	42.841	1.00	17.06		C
ANISOU17749	C	LYS	D	260	2143	2167	2172	27	-27	4	C
ATOM 17750	O	LYS	D	260	94.610	16.067	42.293	1.00	16.73		O
ANISOU17750	O	LYS	D	260	1990	2299	2066	-22	7	-68	O
ATOM 17751	N	TRP	D	261	94.432	18.072	43.231	1.00	15.77		N
ANISOU17751	N	TRP	D	261	1924	2098	1967	-7	-89	18	N
ATOM 17753	CA	TRP	D	261	95.819	18.465	43.060	1.00	14.98		C
ANISOU17753	CA	TRP	D	261	1883	1902	1905	-4	-15	28	C
ATOM 17755	CB	TRP	D	261	95.976	19.981	43.081	1.00	12.87		C
ANISOU17755	CB	TRP	D	261	1558	1643	1688	132	42	-29	C
ATOM 17758	CG	TRP	D	261	95.340	20.621	41.879	1.00	15.22		C
ANISOU17758	CG	TRP	D	261	1959	1919	1905	0	-41	-11	C
ATOM 17759	CD1	TRP	D	261	94.902	20.003	40.728	1.00	15.27		C
ANISOU17759	CD1	TRP	D	261	2001	1779	2020	-11	-133	-16	C
ATOM 17761	NE1	TRP	D	261	94.359	20.932	39.865	1.00	15.73		N
ANISOU17761	NE1	TRP	D	261	2005	1878	2093	-66	-193	2	N
ATOM 17763	CE2	TRP	D	261	94.440	22.170	40.448	1.00	16.18		C
ANISOU17763	CE2	TRP	D	261	2131	1924	2090	1	-65	35	C
ATOM 17764	CD2	TRP	D	261	95.054	22.007	41.715	1.00	14.67		C
ANISOU17764	CD2	TRP	D	261	1869	1776	1926	106	-60	34	C
ATOM 17765	CE3	TRP	D	261	95.273	23.132	42.496	1.00	17.25		C
ANISOU17765	CE3	TRP	D	261	2314	2113	2125	10	63	-32	C
ATOM 17767	CZ3	TRP	D	261	94.836	24.384	42.005	1.00	17.69		C
ANISOU17767	CZ3	TRP	D	261	2413	2221	2085	120	-78	52	C
ATOM 17769	CH2	TRP	D	261	94.226	24.494	40.743	1.00	15.78		C
ANISOU17769	CH2	TRP	D	261	2010	1992	1992	57	-16	-36	C
ATOM 17771	CZ2	TRP	D	261	94.024	23.410	39.964	1.00	14.75		C
ANISOU17771	CZ2	TRP	D	261	1679	1997	1928	43	-196	36	C
ATOM 17773	C	TRP	D	261	96.682	17.840	44.141	1.00	15.05		C
ANISOU17773	C	TRP	D	261	1877	1867	1974	-25	-38	0	C
ATOM 17774	O	TRP	D	261	97.885	17.711	43.972	1.00	16.93		O

ANISOU17774	O	TRP	D	261	2073	2116	2243	-42	-42	-21	O
ATOM 17775	N	ILE	D	262	96.073	17.486	45.252	1.00	14.77		N
ANISOU17775	N	ILE	D	262	1826	1927	1856	55	-18	-71	N
ATOM 17777	CA	ILE	D	262	96.718	16.669	46.275	1.00	15.00		C
ANISOU17777	CA	ILE	D	262	1896	1911	1891	45	2	-50	C
ATOM 17779	CB	ILE	D	262	97.106	17.493	47.502	1.00	14.27		C
ANISOU17779	CB	ILE	D	262	1830	1758	1832	31	45	9	C
ATOM 17781	CG1	ILE	D	262	95.857	18.144	48.129	1.00	13.25		C
ANISOU17781	CG1	ILE	D	262	1696	1646	1689	-6	-18	5	C
ATOM 17784	CD1	ILE	D	262	96.103	18.667	49.538	1.00	12.26		C
ANISOU17784	CD1	ILE	D	262	1379	1655	1625	139	50	44	C
ATOM 17788	CG2	ILE	D	262	98.189	18.517	47.139	1.00	13.17		C
ANISOU17788	CG2	ILE	D	262	1534	1859	1607	21	45	-6	C
ATOM 17792	C	ILE	D	262	95.739	15.557	46.653	1.00	16.33		C
ANISOU17792	C	ILE	D	262	2064	2078	2063	13	-2	-49	C
ATOM 17793	O	ILE	D	262	94.515	15.718	46.498	1.00	16.68		O
ANISOU17793	O	ILE	D	262	2072	2044	2220	44	50	-238	O
ATOM 17794	N	ASP	D	263	96.242	14.416	47.117	1.00	17.84		N
ANISOU17794	N	ASP	D	263	2232	2239	2307	77	48	-52	N
ATOM 17796	CA	ASP	D	263	95.338	13.365	47.591	1.00	18.82		C
ANISOU17796	CA	ASP	D	263	2426	2320	2403	-18	10	-6	C
ATOM 17804	C	ASP	D	263	95.084	13.412	49.102	1.00	18.82		C
ANISOU17804	C	ASP	D	263	2454	2306	2389	-25	13	34	C
ATOM 17805	O	ASP	D	263	95.560	14.281	49.813	1.00	17.56		O
ANISOU17805	O	ASP	D	263	2472	1963	2236	-51	121	101	O
ATOM 17806	N	ALA	D	264	94.351	12.426	49.593	1.00	19.63		N
ANISOU17806	N	ALA	D	264	2507	2425	2525	-110	30	4	N
ATOM 17808	CA	ALA	D	264	93.968	12.370	51.004	1.00	20.08		C
ANISOU17808	CA	ALA	D	264	2587	2521	2522	-68	10	25	C
ATOM 17843	N	LEU	D	267	96.834	15.531	52.289	1.00	19.99		N
ANISOU17843	N	LEU	D	267	2576	2484	2534	12	23	71	N
ATOM 17845	CA	LEU	D	267	96.067	16.442	53.104	1.00	19.90		C
ANISOU17845	CA	LEU	D	267	2522	2537	2501	-16	25	27	C
ATOM 17847	CB	LEU	D	267	94.593	16.385	52.739	1.00	19.42		C
ANISOU17847	CB	LEU	D	267	2472	2431	2475	-61	4	53	C
ATOM 17850	CG	LEU	D	267	93.658	17.235	53.607	1.00	19.49		C
ANISOU17850	CG	LEU	D	267	2454	2522	2429	-28	22	31	C
ATOM 17852	CD1	LEU	D	267	94.029	18.705	53.590	1.00	21.17		C
ANISOU17852	CD1	LEU	D	267	2534	2764	2743	-73	-9	-85	C
ATOM 17856	CD2	LEU	D	267	92.196	17.109	53.157	1.00	19.91		C
ANISOU17856	CD2	LEU	D	267	2471	2624	2470	-116	21	14	C
ATOM 17860	C	LEU	D	267	96.257	16.073	54.562	1.00	20.17		C
ANISOU17860	C	LEU	D	267	2508	2588	2565	15	-52	32	C
ATOM 17861	O	LEU	D	267	96.407	16.963	55.415	1.00	18.12		O
ANISOU17861	O	LEU	D	267	2094	2408	2381	44	-71	78	O
ATOM 17862	N	GLU	D	268	96.236	14.765	54.844	1.00	21.71		N
ANISOU17862	N	GLU	D	268	2704	2758	2784	-16	-32	6	N
ATOM 17903	CB	LEU	D	270	98.474	19.596	54.909	1.00	19.21		C
ANISOU17903	CB	LEU	D	270	2427	2467	2403	-43	89	13	C
ATOM 17906	CG	LEU	D	270	99.194	19.549	53.596	1.00	17.11		C
ANISOU17906	CG	LEU	D	270	2144	2233	2123	50	-68	20	C
ATOM 17908	CD1	LEU	D	270	98.227	20.120	52.556	1.00	13.24		C
ANISOU17908	CD1	LEU	D	270	1475	1738	1816	53	97	-84	C
ATOM 17922	CB	ALA	D	271	95.437	17.753	58.922	1.00	24.84		C
ANISOU17922	CB	ALA	D	271	3193	3201	3043	3	6	-22	C
ATOM 17961	CD1	LEU	D	274	97.816	23.568	58.951	1.00	36.84		C
ANISOU17961	CD1	LEU	D	274	4675	4670	4653	0	-6	-38	C
ATOM 18022	C	GLY	D	278	91.060	24.419	63.113	1.00	27.25		C
ANISOU18022	C	GLY	D	278	3456	3517	3379	-79	89	-9	C
ATOM 18023	O	GLY	D	278	90.308	23.665	62.458	1.00	27.42		O
ANISOU18023	O	GLY	D	278	3486	3598	3331	-191	168	50	O

ATOM 18024	N	TYR D 279	92.119	25.047	62.606	1.00	25.34		N
ANISOU18024	N	TYR D 279	3287	3232	3106	-104	73	3	N
ATOM 18026	CA	TYR D 279	92.493	24.936	61.183	1.00	24.21		C
ANISOU18026	CA	TYR D 279	3097	3090	3008	-94	68	-7	C
ATOM 18028	CB	TYR D 279	93.631	25.928	60.822	1.00	23.42		C
ANISOU18028	CB	TYR D 279	2962	3033	2905	-120	56	15	C
ATOM 18031	CG	TYR D 279	93.758	26.251	59.321	1.00	22.60		C
ANISOU18031	CG	TYR D 279	2924	2826	2837	-46	0	-54	C
ATOM 18032	CD1	TYR D 279	93.176	27.388	58.790	1.00	21.78		C
ANISOU18032	CD1	TYR D 279	2871	2826	2578	3	-31	-117	C
ATOM 18034	CE1	TYR D 279	93.295	27.712	57.459	1.00	20.17		C
ANISOU18034	CE1	TYR D 279	2702	2457	2505	-97	122	-42	C
ATOM 18036	CZ	TYR D 279	94.055	26.880	56.603	1.00	17.34		C
ANISOU18036	CZ	TYR D 279	1973	2258	2358	-167	2	-39	C
ATOM 18037	OH	TYR D 279	94.191	27.182	55.253	1.00	14.53		O
ANISOU18037	OH	TYR D 279	1794	1673	2053	-160	-143	-367	O
ATOM 18039	CE2	TYR D 279	94.655	25.768	57.104	1.00	19.45		C
ANISOU18039	CE2	TYR D 279	2526	2327	2537	-98	66	47	C
ATOM 18041	CD2	TYR D 279	94.533	25.465	58.474	1.00	22.47		C
ANISOU18041	CD2	TYR D 279	3056	2856	2624	-56	-28	-30	C
ATOM 18043	C	TYR D 279	92.874	23.501	60.824	1.00	22.57		C
ANISOU18043	C	TYR D 279	2837	2942	2793	-94	76	30	C
ATOM 18044	O	TYR D 279	92.346	22.952	59.875	1.00	21.48		O
ANISOU18044	O	TYR D 279	2587	2926	2649	-306	280	21	O
ATOM 18045	N	GLY D 280	93.809	22.911	61.546	1.00	22.41		N
ANISOU18045	N	GLY D 280	2822	2920	2770	-82	35	-46	N
ATOM 18047	CA	GLY D 280	94.171	21.525	61.333	1.00	20.97		C
ANISOU18047	CA	GLY D 280	2566	2733	2668	-30	-16	3	C
ATOM 18050	C	GLY D 280	92.992	20.603	61.586	1.00	20.99		C
ANISOU18050	C	GLY D 280	2610	2723	2640	5	4	-26	C
ATOM 18051	O	GLY D 280	92.772	19.640	60.872	1.00	20.50		O
ANISOU18051	O	GLY D 280	2402	2686	2698	-82	-66	-127	O
ATOM 18067	C	GLN D 281	90.114	20.092	61.670	1.00	19.09		C
ANISOU18067	C	GLN D 281	2479	2375	2400	8	-37	37	C
ATOM 18068	O	GLN D 281	89.514	19.113	61.303	1.00	17.44		O
ANISOU18068	O	GLN D 281	2295	2157	2172	58	-66	155	O
ATOM 18069	N	TYR D 282	90.015	21.273	61.048	1.00	18.95		N
ANISOU18069	N	TYR D 282	2487	2323	2390	-18	-42	66	N
ATOM 18071	CA	TYR D 282	89.141	21.440	59.888	1.00	18.11		C
ANISOU18071	CA	TYR D 282	2427	2151	2299	-14	-53	59	C
ATOM 18073	CB	TYR D 282	89.100	22.904	59.461	1.00	18.63		C
ANISOU18073	CB	TYR D 282	2496	2275	2305	-29	-24	39	C
ATOM 18076	CG	TYR D 282	88.325	23.159	58.216	1.00	16.47		C
ANISOU18076	CG	TYR D 282	2127	2014	2115	-27	13	-49	C
ATOM 18077	CD1	TYR D 282	86.975	23.081	58.203	1.00	13.75		C
ANISOU18077	CD1	TYR D 282	1855	1609	1760	15	129	7	C
ATOM 18079	CE1	TYR D 282	86.269	23.346	57.070	1.00	14.20		C
ANISOU18079	CE1	TYR D 282	1953	1719	1721	93	85	-115	C
ATOM 18081	CZ	TYR D 282	86.908	23.699	55.912	1.00	12.49		C
ANISOU18081	CZ	TYR D 282	1726	1330	1689	-169	86	-1	C
ATOM 18082	OH	TYR D 282	86.155	23.976	54.769	1.00	12.84		O
ANISOU18082	OH	TYR D 282	1802	1358	1716	-151	180	-91	O
ATOM 18084	CE2	TYR D 282	88.248	23.800	55.902	1.00	15.47		C
ANISOU18084	CE2	TYR D 282	2068	1804	2006	62	-46	-57	C
ATOM 18086	CD2	TYR D 282	88.962	23.532	57.038	1.00	16.57		C
ANISOU18086	CD2	TYR D 282	2090	2172	2031	-120	-12	47	C
ATOM 18088	C	TYR D 282	89.607	20.570	58.714	1.00	17.79		C
ANISOU18088	C	TYR D 282	2355	2117	2285	-16	-36	71	C
ATOM 18089	O	TYR D 282	88.804	19.857	58.097	1.00	17.64		O
ANISOU18089	O	TYR D 282	2316	2150	2237	1	-253	87	O
ATOM 18090	N	LEU D 283	90.889	20.632	58.400	1.00	17.34		N

ANISOU18090	N	LEU D 283	2348	2022	2216	21	-81	82	N
ATOM 18092	CA	LEU D 283	91.456	19.815	57.342	1.00	17.75		C
ANISOU18092	CA	LEU D 283	2308	2186	2248	5	-15	59	C
ATOM 18094	CB	LEU D 283	92.949	20.073	57.252	1.00	18.08		C
ANISOU18094	CB	LEU D 283	2343	2214	2310	-15	-18	52	C
ATOM 18097	CG	LEU D 283	93.257	21.545	56.902	1.00	19.25		C
ANISOU18097	CG	LEU D 283	2431	2378	2506	36	-31	-6	C
ATOM 18099	CD1	LEU D 283	94.683	21.736	56.613	1.00	20.03		C
ANISOU18099	CD1	LEU D 283	2704	2451	2452	-156	252	-20	C
ATOM 18103	CD2	LEU D 283	92.386	21.975	55.758	1.00	20.46		C
ANISOU18103	CD2	LEU D 283	2868	2539	2365	-40	91	27	C
ATOM 18107	C	LEU D 283	91.194	18.335	57.583	1.00	18.19		C
ANISOU18107	C	LEU D 283	2334	2239	2335	14	-10	-6	C
ATOM 18108	O	LEU D 283	90.792	17.614	56.672	1.00	18.11		O
ANISOU18108	O	LEU D 283	2249	2257	2373	22	-86	-11	O
ATOM 18109	N	LYS D 284	91.412	17.882	58.813	1.00	18.90		N
ANISOU18109	N	LYS D 284	2436	2358	2384	-11	-56	-52	N
ATOM 18111	CA	LYS D 284	91.168	16.483	59.148	1.00	19.62		C
ANISOU18111	CA	LYS D 284	2500	2474	2480	-15	-21	46	C
ATOM 18129	C	LYS D 284	89.711	16.096	58.853	1.00	18.87		C
ANISOU18129	C	LYS D 284	2408	2416	2343	-23	-5	97	C
ATOM 18130	O	LYS D 284	89.434	15.041	58.326	1.00	18.01		O
ANISOU18130	O	LYS D 284	2157	2408	2275	-56	-183	209	O
ATOM 18131	N	ARG D 285	88.795	16.972	59.157	1.00	19.11		N
ANISOU18131	N	ARG D 285	2455	2414	2389	-68	29	142	N
ATOM 18133	CA	ARG D 285	87.371	16.667	58.959	1.00	20.61		C
ANISOU18133	CA	ARG D 285	2598	2582	2649	-34	-54	78	C
ATOM 18135	CB	ARG D 285	86.549	17.732	59.630	1.00	20.85		C
ANISOU18135	CB	ARG D 285	2642	2644	2635	-66	27	116	C
ATOM 18138	CG	ARG D 285	85.138	17.618	59.292	1.00	25.19		C
ANISOU18138	CG	ARG D 285	3069	3231	3269	-45	-153	97	C
ATOM 18141	CD	ARG D 285	84.180	18.252	60.283	1.00	30.00		C
ANISOU18141	CD	ARG D 285	3779	3893	3724	-27	144	-66	C
ATOM 18144	NE	ARG D 285	84.349	19.686	60.519	1.00	34.32		N
ANISOU18144	NE	ARG D 285	4520	4113	4407	-3	25	23	N
ATOM 18146	CZ	ARG D 285	83.705	20.659	59.857	1.00	34.86		C
ANISOU18146	CZ	ARG D 285	4439	4306	4499	74	-57	9	C
ATOM 18147	NH1	ARG D 285	82.860	20.373	58.857	1.00	36.54		N
ANISOU18147	NH1	ARG D 285	4712	4548	4623	8	-96	-70	N
ATOM 18150	NH2	ARG D 285	83.930	21.922	60.196	1.00	32.17		N
ANISOU18150	NH2	ARG D 285	4010	4047	4165	46	18	93	N
ATOM 18153	C	ARG D 285	86.964	16.490	57.486	1.00	20.79		C
ANISOU18153	C	ARG D 285	2599	2589	2711	1	-64	84	C
ATOM 18154	O	ARG D 285	86.068	15.697	57.138	1.00	20.29		O
ANISOU18154	O	ARG D 285	2554	2412	2743	17	-124	226	O
ATOM 18155	N	LEU D 286	87.619	17.237	56.617	1.00	21.21		N
ANISOU18155	N	LEU D 286	2578	2699	2778	7	-3	46	N
ATOM 18157	CA	LEU D 286	87.355	17.160	55.198	1.00	22.40		C
ANISOU18157	CA	LEU D 286	2755	2893	2862	9	-48	14	C
ATOM 18159	CB	LEU D 286	88.129	18.232	54.469	1.00	23.39		C
ANISOU18159	CB	LEU D 286	2962	3021	2901	-26	-58	43	C
ATOM 18162	CG	LEU D 286	87.681	19.636	54.863	1.00	25.94		C
ANISOU18162	CG	LEU D 286	3348	3313	3194	33	-13	-44	C
ATOM 18164	CD1	LEU D 286	88.501	20.677	54.176	1.00	28.20		C
ANISOU18164	CD1	LEU D 286	3695	3574	3442	-69	117	-3	C
ATOM 18168	CD2	LEU D 286	86.203	19.889	54.562	1.00	28.64		C
ANISOU18168	CD2	LEU D 286	3530	3777	3573	22	-24	-16	C
ATOM 18172	C	LEU D 286	87.696	15.808	54.610	1.00	22.57		C
ANISOU18172	C	LEU D 286	2832	2849	2894	-50	-49	55	C
ATOM 18173	O	LEU D 286	87.313	15.491	53.464	1.00	22.32		O
ANISOU18173	O	LEU D 286	2816	2811	2850	-59	-179	190	O

ATOM 18174	N	LEU D 287	88.452	15.010	55.359	1.00	22.09		N
ANISOU18174	N	LEU D 287	2744	2842	2806	-63	-72	63	N
ATOM 18176	CA	LEU D 287	88.773	13.681	54.898	1.00	22.67		C
ANISOU18176	CA	LEU D 287	2839	2889	2883	-13	-39	46	C
ATOM 18178	CB	LEU D 287	89.993	13.094	55.628	1.00	22.85		C
ANISOU18178	CB	LEU D 287	2807	2982	2893	-29	-39	10	C
ATOM 18181	CG	LEU D 287	91.373	13.739	55.405	1.00	24.06		C
ANISOU18181	CG	LEU D 287	3050	3066	3022	-28	54	13	C
ATOM 18183	CD1	LEU D 287	92.298	13.241	56.508	1.00	25.08		C
ANISOU18183	CD1	LEU D 287	3085	3226	3217	23	-2	-92	C
ATOM 18187	CD2	LEU D 287	91.958	13.463	54.022	1.00	23.08		C
ANISOU18187	CD2	LEU D 287	3004	2752	3012	42	65	-33	C
ATOM 18191	C	LEU D 287	87.601	12.727	55.102	1.00	22.23		C
ANISOU18191	C	LEU D 287	2758	2830	2854	-18	-115	33	C
ATOM 18192	O	LEU D 287	87.513	11.753	54.355	1.00	23.01		O
ANISOU18192	O	LEU D 287	2829	2751	3159	0	-225	72	O
ATOM 18193	N	THR D 288	86.759	13.000	56.103	1.00	21.67		N
ANISOU18193	N	THR D 288	2648	2721	2862	25	-94	72	N
ATOM 18195	CA	THR D 288	85.638	12.117	56.519	1.00	22.58		C
ANISOU18195	CA	THR D 288	2735	2881	2961	33	-39	44	C
ATOM 18205	C	THR D 288	84.226	12.700	56.347	1.00	21.40		C
ANISOU18205	C	THR D 288	2644	2710	2777	29	3	69	C
ATOM 18207	N	GLU D 289	84.105	13.745	55.558	1.00	19.74		N
ANISOU18207	N	GLU D 289	2473	2502	2525	12	-51	-33	N
ATOM 18209	CA	GLU D 289	82.828	14.362	55.343	1.00	17.87		C
ANISOU18209	CA	GLU D 289	2272	2231	2287	38	34	-28	C
ATOM 18211	CB	GLU D 289	82.766	15.696	56.107	1.00	18.82		C
ANISOU18211	CB	GLU D 289	2390	2431	2330	26	2	-71	C
ATOM 18214	CG	GLU D 289	81.337	16.241	56.183	1.00	18.36		C
ANISOU18214	CG	GLU D 289	2264	2363	2347	97	-24	14	C
ATOM 18217	CD	GLU D 289	81.227	17.667	56.736	1.00	21.02		C
ANISOU18217	CD	GLU D 289	2657	2548	2782	14	67	-123	C
ATOM 18218	OE1	GLU D 289	82.274	18.358	56.890	1.00	21.45		O
ANISOU18218	OE1	GLU D 289	2894	2412	2844	60	27	-240	O
ATOM 18219	OE2	GLU D 289	80.077	18.072	57.035	1.00	20.60		O
ANISOU18219	OE2	GLU D 289	2730	2234	2862	267	-193	-62	O
ATOM 18220	C	GLU D 289	82.649	14.675	53.875	1.00	16.22		C
ANISOU18220	C	GLU D 289	2045	2026	2092	60	31	-67	C
ATOM 18221	O	GLU D 289	83.540	15.259	53.285	1.00	17.47		O
ANISOU18221	O	GLU D 289	2238	2379	2018	136	117	-36	O
ATOM 18222	N	THR D 290	81.483	14.377	53.311	1.00	14.59		N
ANISOU18222	N	THR D 290	2002	1752	1787	75	63	-80	N
ATOM 18224	CA	THR D 290	81.146	14.822	51.957	1.00	13.30		C
ANISOU18224	CA	THR D 290	1647	1658	1746	75	-14	-51	C
ATOM 18226	CB	THR D 290	80.161	13.848	51.295	1.00	14.18		C
ANISOU18226	CB	THR D 290	1765	1796	1825	82	-59	-42	C
ATOM 18228	OG1	THR D 290	80.799	12.597	51.037	1.00	17.72		O
ANISOU18228	OG1	THR D 290	2105	2207	2419	218	-134	-90	O
ATOM 18230	CG2	THR D 290	79.717	14.347	49.896	1.00	12.57		C
ANISOU18230	CG2	THR D 290	1738	1468	1571	14	-52	-140	C
ATOM 18234	C	THR D 290	80.562	16.236	52.014	1.00	11.49		C
ANISOU18234	C	THR D 290	1395	1542	1426	27	-72	35	C
ATOM 18235	O	THR D 290	79.590	16.506	52.708	1.00	11.72		O
ANISOU18235	O	THR D 290	1425	1606	1421	98	-79	8	O
ATOM 18236	N	VAL D 291	81.150	17.146	51.287	1.00	10.13		N
ANISOU18236	N	VAL D 291	1134	1369	1345	49	-2	-13	N
ATOM 18238	CA	VAL D 291	80.644	18.529	51.242	1.00	9.71		C
ANISOU18238	CA	VAL D 291	1100	1329	1257	53	55	-1	C
ATOM 18240	CB	VAL D 291	81.703	19.569	51.742	1.00	9.58		C
ANISOU18240	CB	VAL D 291	1141	1260	1238	-17	107	22	C
ATOM 18242	CG1	VAL D 291	81.217	20.975	51.614	1.00	8.64		C

ANISOU18242	CG1	VAL	D	291	836	1313	1133	78	-53	-33	C
ATOM 18246	CG2	VAL	D	291	82.095	19.345	53.170	1.00	11.02		C
ANISOU18246	CG2	VAL	D	291	1128	1557	1501	107	-119	114	C
ATOM 18250	C	VAL	D	291	80.279	18.802	49.801	1.00	9.92		C
ANISOU18250	C	VAL	D	291	1203	1354	1211	50	99	-42	C
ATOM 18251	O	VAL	D	291	81.154	18.725	48.913	1.00	10.32		O
ANISOU18251	O	VAL	D	291	1203	1531	1185	248	236	-49	O
ATOM 18252	N	TYR	D	292	79.017	19.143	49.573	1.00	9.62		N
ANISOU18252	N	TYR	D	292	1168	1316	1169	104	113	-82	N
ATOM 18254	CA	TYR	D	292	78.475	19.404	48.268	1.00	11.45		C
ANISOU18254	CA	TYR	D	292	1482	1464	1406	44	42	-28	C
ATOM 18256	CB	TYR	D	292	76.973	19.151	48.270	1.00	10.83		C
ANISOU18256	CB	TYR	D	292	1432	1373	1307	52	15	-49	C
ATOM 18259	CG	TYR	D	292	76.646	17.772	48.695	1.00	9.96		C
ANISOU18259	CG	TYR	D	292	1181	1427	1175	201	-118	145	C
ATOM 18260	CD1	TYR	D	292	75.959	17.543	49.874	1.00	8.91		C
ANISOU18260	CD1	TYR	D	292	889	1317	1177	231	-81	171	C
ATOM 18262	CE1	TYR	D	292	75.687	16.273	50.262	1.00	11.78		C
ANISOU18262	CE1	TYR	D	292	1526	1419	1530	79	70	128	C
ATOM 18264	CZ	TYR	D	292	76.016	15.181	49.462	1.00	11.39		C
ANISOU18264	CZ	TYR	D	292	1326	1522	1478	76	85	56	C
ATOM 18265	OH	TYR	D	292	75.731	13.914	49.954	1.00	13.39		O
ANISOU18265	OH	TYR	D	292	1607	1473	2007	101	-64	-61	O
ATOM 18267	CE2	TYR	D	292	76.678	15.369	48.297	1.00	12.20		C
ANISOU18267	CE2	TYR	D	292	1721	1559	1355	81	-3	71	C
ATOM 18269	CD2	TYR	D	292	76.988	16.684	47.904	1.00	10.05		C
ANISOU18269	CD2	TYR	D	292	1216	1386	1214	115	-10	-21	C
ATOM 18271	C	TYR	D	292	78.728	20.820	47.802	1.00	13.53		C
ANISOU18271	C	TYR	D	292	1873	1610	1657	91	12	12	C
ATOM 18272	O	TYR	D	292	78.566	21.015	46.594	1.00	15.36		O
ANISOU18272	O	TYR	D	292	2248	1872	1713	176	202	79	O
ATOM 18273	OXT	TYR	D	292	79.058	21.621	48.661	1.00	15.02		O
ANISOU18273	OXT	TYR	D	292	2059	1782	1863	34	-29	0	O
ATOM 20579	CA	ASP	E	150	63.835	16.845	36.379	1.00	19.75		C
ANISOU20579	CA	ASP	E	150	2540	2527	2437	3	-14	6	C
ATOM 20581	CB	ASP	E	150	63.521	16.810	37.882	1.00	20.77		C
ANISOU20581	CB	ASP	E	150	2749	2620	2521	70	79	-40	C
ATOM 20584	CG	ASP	E	150	63.222	15.432	38.415	1.00	22.96		C
ANISOU20584	CG	ASP	E	150	3132	2829	2761	26	86	51	C
ATOM 20586	OD2	ASP	E	150	62.722	15.336	39.552	1.00	25.38		O
ANISOU20586	OD2	ASP	E	150	3636	3229	2775	127	317	-44	O
ATOM 20587	C	ASP	E	150	64.974	15.900	36.017	1.00	20.35		C
ANISOU20587	C	ASP	E	150	2568	2657	2504	23	45	-20	C
ATOM 20589	N	GLN	E	151	66.107	16.073	36.678	1.00	20.64		N
ANISOU20589	N	GLN	E	151	2648	2777	2417	-32	-52	10	N
ATOM 20591	CA	GLN	E	151	67.290	15.291	36.326	1.00	23.23		C
ANISOU20591	CA	GLN	E	151	2962	2987	2875	56	-32	-9	C
ATOM 20593	CB	GLN	E	151	68.504	15.758	37.101	1.00	23.58		C
ANISOU20593	CB	GLN	E	151	2919	3098	2943	-42	16	62	C
ATOM 20596	CG	GLN	E	151	68.711	17.163	36.846	1.00	28.43		C
ANISOU20596	CG	GLN	E	151	3741	3461	3599	30	-11	-20	C
ATOM 20599	CD	GLN	E	151	70.085	17.584	37.124	1.00	33.30		C
ANISOU20599	CD	GLN	E	151	3986	4277	4387	-132	-1	43	C
ATOM 20600	OE1	GLN	E	151	71.014	16.757	37.168	1.00	36.56		O
ANISOU20600	OE1	GLN	E	151	4755	4289	4848	64	2	78	O
ATOM 20601	NE2	GLN	E	151	70.257	18.885	37.324	1.00	37.87		N
ANISOU20601	NE2	GLN	E	151	4946	4495	4947	32	-30	4	N
ATOM 20604	C	GLN	E	151	67.102	13.822	36.530	1.00	23.67		C
ANISOU20604	C	GLN	E	151	2983	3057	2952	33	-25	29	C
ATOM 20605	O	GLN	E	151	67.744	12.989	35.856	1.00	25.73		O
ANISOU20605	O	GLN	E	151	3298	3266	3213	198	23	-17	O

ATOM 20606	N	GLY E 152	66.210	13.483	37.432	1.00	23.38		N
ANISOU20606	N	GLY E 152	2949	3023	2911	89	-43	-7	N
ATOM 36741	C1,	TDG M 600	69.071	40.140	46.254	1.00	12.52		C
ANISOU36741	C1,	TDG M 600	1652	1528	1577	-43	-40	48	C
ATOM 36743	C2,	TDG M 600	68.642	38.804	45.927	1.00	12.49		C
ANISOU36743	C2,	TDG M 600	1848	1479	1417	119	-135	46	C
ATOM 36746	O4,	TDG M 600	70.367	40.187	45.700	1.00	12.98		O
ANISOU36746	O4,	TDG M 600	1631	1743	1557	-35	-110	31	O
ATOM 36747	C4,	TDG M 600	70.895	38.888	45.554	1.00	12.38		C
ANISOU36747	C4,	TDG M 600	1599	1681	1422	-47	31	68	C
ATOM 36749	C3,	TDG M 600	69.814	37.853	45.978	1.00	11.39		C
ANISOU36749	C3,	TDG M 600	1283	1383	1661	-210	-54	6	C
ATOM 36751	O3,	TDG M 600	70.084	37.467	47.319	1.00	13.06		O
ANISOU36751	O3,	TDG M 600	1517	1915	1528	101	89	66	O
ATOM 36753	C5,	TDG M 600	71.471	38.716	44.170	1.00	10.61		C
ANISOU36753	C5,	TDG M 600	1263	1301	1468	-252	-2	231	C
ATOM 36756	O5,	TDG M 600	70.401	38.888	43.273	1.00	11.41		O
ANISOU36756	O5,	TDG M 600	1494	1490	1351	116	32	379	O
ATOM 36757	P	TDG M 600	70.149	37.834	42.076	1.00	12.32		P
ANISOU36757	P	TDG M 600	1732	1567	1380	122	122	152	P
ATOM 36758	O1P	TDG M 600	69.289	38.482	40.969	1.00	14.76		O
ANISOU36758	O1P	TDG M 600	1613	2073	1919	33	-276	224	O
ATOM 36759	O2P	TDG M 600	69.742	36.452	42.561	1.00	12.62		O
ANISOU36759	O2P	TDG M 600	1535	1558	1699	-136	71	123	O
ATOM 36760	OPP	TDG M 600	71.627	37.565	41.456	1.00	12.91		O
ANISOU36760	OPP	TDG M 600	1878	1484	1543	0	238	219	O
ATOM 36761	P2	TDG M 600	72.743	38.612	40.959	1.00	12.98		P
ANISOU36761	P2	TDG M 600	1503	1763	1663	-113	251	-83	P
ATOM 36762	O3P	TDG M 600	74.118	38.290	41.621	1.00	14.23		O
ANISOU36762	O3P	TDG M 600	1998	1597	1812	16	138	133	O
ATOM 36763	O4P	TDG M 600	72.259	40.106	40.978	1.00	14.72		O
ANISOU36763	O4P	TDG M 600	2204	1690	1699	-71	320	553	O
ATOM 36764	O1	TDG M 600	72.876	38.100	39.426	1.00	12.82		O
ANISOU36764	O1	TDG M 600	1910	1383	1577	-94	0	233	O
ATOM 36765	C1	TDG M 600	72.000	38.634	38.397	1.00	13.50		C
ANISOU36765	C1	TDG M 600	1534	1903	1692	-41	-259	68	C
ATOM 36767	C2	TDG M 600	71.560	37.546	37.444	1.00	14.62		C
ANISOU36767	C2	TDG M 600	1975	1745	1836	58	-112	40	C
ATOM 36769	O2	TDG M 600	70.988	36.403	38.131	1.00	18.41		O
ANISOU36769	O2	TDG M 600	2442	2521	2032	-394	203	-72	O
ATOM 36771	C3	TDG M 600	72.716	37.132	36.563	1.00	13.69		C
ANISOU36771	C3	TDG M 600	1492	1916	1792	82	-86	-16	C
ATOM 36773	O3	TDG M 600	72.247	36.256	35.535	1.00	16.32		O
ANISOU36773	O3	TDG M 600	1480	2450	2270	294	-62	-18	O
ATOM 36775	C4	TDG M 600	73.471	38.309	35.953	1.00	16.71		C
ANISOU36775	C4	TDG M 600	2150	2149	2048	12	34	30	C
ATOM 36777	O4	TDG M 600	74.652	37.783	35.244	1.00	16.79		O
ANISOU36777	O4	TDG M 600	2094	2001	2283	-101	122	-37	O
ATOM 36779	C5	TDG M 600	73.968	39.273	37.062	1.00	17.56		C
ANISOU36779	C5	TDG M 600	2392	2141	2139	-70	54	-1	C
ATOM 36781	O5	TDG M 600	72.923	39.661	37.942	1.00	15.41		O
ANISOU36781	O5	TDG M 600	2084	1974	1797	-178	-205	82	O
ATOM 36967	O41	TDG Q 600	86.862	24.808	48.956	1.00	16.34		O
ANISOU36967	O41	TDG Q 600	2009	1872	2327	45	256	262	O
ATOM 36968	C41	TDG Q 600	86.276	25.942	48.639	1.00	16.13		C
ANISOU36968	C41	TDG Q 600	1640	2189	2299	46	218	30	C
ATOM 36969	N31	TDG Q 600	86.639	27.024	49.319	1.00	17.72		N
ANISOU36969	N31	TDG Q 600	2177	2254	2303	47	101	121	N
ATOM 36971	C21	TDG Q 600	86.068	28.205	49.065	1.00	17.09		C
ANISOU36971	C21	TDG Q 600	1981	2256	2254	174	-22	-93	C
ATOM 36972	O21	TDG Q 600	86.490	29.234	49.737	1.00	17.42		O

ANISOU36972	O21	TDG	Q	600	1931	2032	2656	169	-225	67	O
ATOM 36973	C51	TDG	Q	600	85.288	26.008	47.681	1.00	16.19		C
ANISOU36973	C51	TDG	Q	600	2079	2108	1962	-32	163	78	C
ATOM 36974	C5A	TDG	Q	600	84.884	24.753	46.957	1.00	19.08		C
ANISOU36974	C5A	TDG	Q	600	2282	2282	2682	11	-11	36	C
ATOM 36978	C61	TDG	Q	600	84.680	27.239	47.456	1.00	15.21		C
ANISOU36978	C61	TDG	Q	600	1540	2281	1957	57	-80	-16	C
ATOM 36980	N11	TDG	Q	600	85.096	28.329	48.129	1.00	14.21		N
ANISOU36980	N11	TDG	Q	600	1665	1752	1981	123	50	68	N
ATOM 36981	C1,	TDG	Q	600	84.476	29.626	47.985	1.00	12.97		C
ANISOU36981	C1,	TDG	Q	600	1608	1754	1564	64	-35	-22	C
ATOM 36983	C2,	TDG	Q	600	84.517	29.998	46.571	1.00	10.65		C
ANISOU36983	C2,	TDG	Q	600	1207	1271	1569	49	155	188	C
ATOM 36986	O4,	TDG	Q	600	83.070	29.500	48.222	1.00	15.58		O
ANISOU36986	O4,	TDG	Q	600	2004	1706	2210	69	92	176	O
ATOM 36987	C4,	TDG	Q	600	82.335	30.200	47.183	1.00	10.85		C
ANISOU36987	C4,	TDG	Q	600	1307	1505	1307	-52	194	-107	C
ATOM 36989	C3,	TDG	Q	600	83.333	30.876	46.174	1.00	10.14		C
ANISOU36989	C3,	TDG	Q	600	1002	1414	1435	-142	114	134	C
ATOM 36991	O3,	TDG	Q	600	83.442	32.199	46.606	1.00	12.71		O
ANISOU36991	O3,	TDG	Q	600	1015	1589	2223	71	320	-98	O
ATOM 36993	C5,	TDG	Q	600	81.323	29.283	46.569	1.00	11.47		C
ANISOU36993	C5,	TDG	Q	600	1290	1667	1398	334	-350	396	C
ATOM 36996	O5,	TDG	Q	600	81.940	28.227	45.894	1.00	14.18		O
ANISOU36996	O5,	TDG	Q	600	1581	1785	2022	-282	91	-1	O
ATOM 36997	P	TDG	Q	600	81.448	27.903	44.409	1.00	16.76		P
ANISOU36997	P	TDG	Q	600	1786	2425	2154	-17	19	101	P
ATOM 36998	O1P	TDG	Q	600	82.020	26.443	44.163	1.00	18.61		O
ANISOU36998	O1P	TDG	Q	600	2672	2271	2128	42	149	159	O
ATOM 36999	O2P	TDG	Q	600	81.711	29.039	43.369	1.00	17.08		O
ANISOU36999	O2P	TDG	Q	600	2134	1997	2359	-108	-77	-137	O
ATOM 37000	OPP	TDG	Q	600	79.802	27.834	44.549	1.00	13.41		O
ANISOU37000	OPP	TDG	Q	600	1535	1777	1783	124	-55	32	O
ATOM 37001	P2	TDG	Q	600	78.855	27.029	45.563	1.00	15.84		P
ANISOU37001	P2	TDG	Q	600	2054	2158	1805	96	-199	-11	P
ATOM 37002	O3P	TDG	Q	600	77.787	28.041	46.105	1.00	13.69		O
ANISOU37002	O3P	TDG	Q	600	1685	1849	1667	-127	-195	88	O
ATOM 37003	O4P	TDG	Q	600	79.656	26.000	46.445	1.00	18.24		O
ANISOU37003	O4P	TDG	Q	600	2327	2364	2237	115	-245	18	O
ATOM 37004	O1	TDG	Q	600	78.002	26.083	44.500	1.00	14.18		O
ANISOU37004	O1	TDG	Q	600	1916	1811	1659	-94	-4	265	O
ATOM 37005	C1	TDG	Q	600	78.429	24.770	44.050	1.00	16.67		C
ANISOU37005	C1	TDG	Q	600	2129	1958	2245	59	81	-80	C
ATOM 37007	C2	TDG	Q	600	78.121	24.558	42.619	1.00	18.04		C
ANISOU37007	C2	TDG	Q	600	2317	2135	2402	20	-13	47	C
ATOM 37009	O2	TDG	Q	600	78.792	25.524	41.827	1.00	19.74		O
ANISOU37009	O2	TDG	Q	600	2413	2320	2765	-162	53	-41	O
ATOM 37011	C3	TDG	Q	600	76.604	24.563	42.375	1.00	17.10		C
ANISOU37011	C3	TDG	Q	600	2163	2060	2272	-52	46	-34	C
ATOM 37013	O3	TDG	Q	600	76.444	24.130	41.027	1.00	16.67		O
ANISOU37013	O3	TDG	Q	600	1910	2067	2354	-46	-23	26	O
ATOM 37015	C4	TDG	Q	600	75.983	23.542	43.320	1.00	17.79		C
ANISOU37015	C4	TDG	Q	600	2378	2019	2360	123	70	82	C
ATOM 37017	O4	TDG	Q	600	74.571	23.410	43.131	1.00	20.12		O
ANISOU37017	O4	TDG	Q	600	2672	2103	2867	-362	-46	10	O
ATOM 37019	C5	TDG	Q	600	76.263	23.940	44.759	1.00	18.99		C
ANISOU37019	C5	TDG	Q	600	2496	2241	2477	-59	1	135	C
ATOM 37021	O5	TDG	Q	600	77.649	24.013	44.971	1.00	18.79		O
ANISOU37021	O5	TDG	Q	600	2468	2220	2448	-55	206	-98	O
ATOM 37022	C6	TDG	Q	600	75.801	22.898	45.774	1.00	18.41		C
ANISOU37022	C6	TDG	Q	600	2330	2269	2396	72	237	62	C

ATOM 37025	O6	TDG Q 600	76.267	21.596	45.472	1.00	17.18		O
ANISOU37025	O6	TDG Q 600	2665	1570	2292	-282	186	104	O
ATOM 37548	S	SO4 J 1	72.371	26.539	41.932	1.00	43.95		S
ANISOU37548	S	SO4 J 1	5527	5558	5611	-21	-109	13	S
ATOM 37549	O1	SO4 J 1	73.643	25.829	42.171	1.00	40.90		O
ANISOU37549	O1	SO4 J 1	5221	4857	5461	-37	-94	-162	O
ATOM 37550	O2	SO4 J 1	72.568	27.564	40.840	1.00	42.62		O
ANISOU37550	O2	SO4 J 1	5535	5405	5252	1	-10	15	O
ATOM 37551	O3	SO4 J 1	71.309	25.587	41.707	1.00	41.68		O
ANISOU37551	O3	SO4 J 1	5399	5239	5198	-65	-230	-11	O
ATOM 37552	O4	SO4 J 1	71.974	27.257	43.160	1.00	42.60		O
ANISOU37552	O4	SO4 J 1	5240	5559	5387	33	-10	13	O
ATOM 37581	O	HOH I 7	77.730	22.240	50.912	1.00	16.46		O
ANISOU37581	O	HOH I 7	2098	1901	2253	321	358	260	O
ATOM 37599	O	HOH I 13	87.886	42.778	36.972	1.00	14.12		O
ANISOU37599	O	HOH I 13	1727	1858	1779	693	-111	-101	O
ATOM 37614	O	HOH I 18	75.994	24.384	51.895	1.00	11.33		O
ANISOU37614	O	HOH I 18	1664	1593	1047	-215	167	-22	O
ATOM 37659	O	HOH I 33	76.692	34.694	46.646	1.00	11.31		O
ANISOU37659	O	HOH I 33	1421	1813	1061	144	-334	5	O
ATOM 37668	O	HOH I 36	76.863	26.212	53.757	1.00	9.98		O
ANISOU37668	O	HOH I 36	1199	1323	1268	-66	-33	170	O
ATOM 37701	O	HOH I 47	77.668	16.261	56.572	1.00	20.19		O
ANISOU37701	O	HOH I 47	2668	2473	2530	119	84	212	O
ATOM 37737	O	HOH I 59	73.167	25.841	45.314	1.00	13.31		O
ANISOU37737	O	HOH I 59	1662	2103	1291	6	178	-184	O
ATOM 37836	O	HOH I 92	63.163	21.494	43.620	1.00	15.08		O
ANISOU37836	O	HOH I 92	2002	1638	2088	-275	179	135	O
ATOM 37893	O	HOH I 111	68.277	37.809	49.089	1.00	14.09		O
ANISOU37893	O	HOH I 111	1653	2108	1591	-90	-116	320	O
ATOM 37896	O	HOH I 112	78.713	24.362	48.362	1.00	15.00		O
ANISOU37896	O	HOH I 112	1666	1943	2089	70	190	216	O
ATOM 37899	O	HOH I 113	77.609	45.126	43.459	1.00	11.10		O
ANISOU37899	O	HOH I 113	2133	1070	1014	-6	199	258	O
ATOM 37941	O	HOH I 127	85.710	45.011	53.303	1.00	17.31		O
ANISOU37941	O	HOH I 127	2409	2218	1948	107	-18	122	O
ATOM 38031	O	HOH I 157	74.336	12.788	54.780	1.00	17.23		O
ANISOU38031	O	HOH I 157	1791	2331	2422	478	-145	-180	O
ATOM 38037	O	HOH I 159	97.934	26.920	56.050	1.00	21.51		O
ANISOU38037	O	HOH I 159	2077	3012	3082	-232	-321	252	O
ATOM 38040	O	HOH I 160	83.513	16.448	49.990	1.00	21.25		O
ANISOU38040	O	HOH I 160	2658	2390	3022	328	215	248	O
ATOM 38055	O	HOH I 165	77.473	37.866	37.791	1.00	14.84		O
ANISOU38055	O	HOH I 165	1919	1734	1986	-76	-88	59	O
ATOM 38061	O	HOH I 167	88.096	26.769	51.687	1.00	13.74		O
ANISOU38061	O	HOH I 167	1133	2049	2038	109	106	333	O
ATOM 38064	O	HOH I 168	64.424	24.683	52.860	1.00	13.22		O
ANISOU38064	O	HOH I 168	1669	2056	1298	113	54	-362	O
ATOM 38121	O	HOH I 187	83.144	28.702	51.970	1.00	19.82		O
ANISOU38121	O	HOH I 187	2962	1996	2572	255	-597	-100	O
ATOM 38181	O	HOH I 207	88.691	35.310	48.169	1.00	20.46		O
ANISOU38181	O	HOH I 207	2073	3421	2278	58	-446	20	O
ATOM 38253	O	HOH I 231	85.979	33.047	47.066	1.00	16.89		O
ANISOU38253	O	HOH I 231	2094	1912	2408	54	23	-14	O
ATOM 38331	O	HOH I 257	64.201	23.448	41.992	1.00	20.24		O
ANISOU38331	O	HOH I 257	2311	2539	2840	198	-138	27	O
ATOM 38352	O	HOH I 264	81.992	22.886	48.432	1.00	17.31		O
ANISOU38352	O	HOH I 264	2606	2029	1940	-129	-99	-125	O
ATOM 38451	O	HOH I 297	65.761	15.182	46.292	1.00	22.59		O
ANISOU38451	O	HOH I 297	2699	2454	3430	-89	-154	-355	O
ATOM 38478	O	HOH I 306	65.697	25.417	43.115	1.00	19.42		O

ANISOU38478	O	HOH I 306	2937	2136	2306	435	314	-132	O
ATOM 38529	O	HOH I 323	90.221	36.889	46.346	1.00	20.41		O
ANISOU38529	O	HOH I 323	2545	2561	2648	242	162	-55	O
ATOM 38832	O	HOH I 424	63.087	22.268	39.278	1.00	30.72		O
ANISOU38832	O	HOH I 424	3920	3965	3785	-47	-262	-127	O
ATOM 38919	O	HOH I 453	67.715	17.228	44.363	1.00	27.90		O
ANISOU38919	O	HOH I 453	3496	3862	3240	-373	-149	-234	O
ATOM 38934	O	HOH I 458	81.354	24.361	46.004	1.00	24.09		O
ANISOU38934	O	HOH I 458	3127	3187	2836	200	-243	-86	O
ATOM 38964	O	HOH I 468	73.471	33.889	35.812	1.00	24.60		O
ANISOU38964	O	HOH I 468	3640	2438	3268	95	225	-62	O
ATOM 38970	O	HOH I 470	76.522	33.034	37.156	1.00	29.47		O
ANISOU38970	O	HOH I 470	4063	3727	3407	29	107	-115	O
ATOM 39081	O	HOH I 507	71.335	20.178	44.538	1.00	23.63		O
ANISOU39081	O	HOH I 507	2776	3352	2848	-92	231	-295	O
ATOM 39195	O	HOH I 545	76.135	35.410	36.289	1.00	28.45		O
ANISOU39195	O	HOH I 545	3443	3957	3407	5	-43	513	O
ATOM 39252	O	HOH I 564	71.034	23.217	43.996	1.00	31.12		O
ANISOU39252	O	HOH I 564	4381	3738	3704	-191	153	-264	O
ATOM 39534	O	HOH I 658	79.531	12.996	54.737	1.00	23.78		O
ANISOU39534	O	HOH I 658	2826	2973	3237	4	20	327	O
ATOM 39546	O	HOH I 662	78.450	38.008	34.360	1.00	35.27		O
ANISOU39546	O	HOH I 662	4760	4563	4078	-312	155	-140	O
ATOM 39555	O	HOH I 665	65.184	29.767	37.286	1.00	26.86		O
ANISOU39555	O	HOH I 665	3320	3655	3230	-534	-36	138	O
ATOM 39600	O	HOH I 680	68.064	27.091	39.320	1.00	30.93		O
ANISOU39600	O	HOH I 680	3898	4393	3460	268	-136	-90	O
ATOM 39795	O	HOH I 745	65.311	17.380	42.990	0.00	29.76		O
ANISOU39795	O	HOH I 745	3657	3838	3814	-15	122	60	O
ATOM 39798	O	HOH I 746	73.979	20.306	44.028	1.00	33.29		O
ANISOU39798	O	HOH I 746	4033	4481	4134	-145	278	-264	O
ATOM 39810	O	HOH I 750	82.632	29.387	54.649	1.00	21.70		O
ANISOU39810	O	HOH I 750	2273	2644	3327	-171	-296	149	O
ATOM 39849	O	HOH I 763	76.456	11.744	48.843	1.00	29.61		O
ANISOU39849	O	HOH I 763	3768	3512	3968	-302	-130	-155	O
ATOM 39864	O	HOH I 768	75.026	25.830	39.829	1.00	31.65		O
ANISOU39864	O	HOH I 768	4316	3653	4056	-94	-213	-49	O
ATOM 39897	O	HOH I 779	76.219	13.476	52.729	1.00	25.96		O
ANISOU39897	O	HOH I 779	2493	3855	3514	235	390	-200	O
ATOM 40059	O	HOH I 833	80.573	21.969	45.066	1.00	24.01		O
ANISOU40059	O	HOH I 833	3003	3043	3073	235	142	-17	O
ATOM 40074	O	HOH I 838	87.060	27.226	37.189	1.00	33.33		O
ANISOU40074	O	HOH I 838	4406	4189	4067	152	-96	-109	O
ATOM 40128	O	HOH I 856	77.486	12.237	46.550	1.00	34.07		O
ANISOU40128	O	HOH I 856	3948	4240	4755	3	103	-123	O
ATOM 40353	O	HOH I 931	67.083	29.743	35.307	1.00	38.75		O
ANISOU40353	O	HOH I 931	4740	5143	4841	-97	-162	-50	O
ATOM 40356	O	HOH I 932	79.944	21.840	60.235	1.00	29.91		O
ANISOU40356	O	HOH I 932	3908	3445	4011	86	18	114	O
ATOM 40434	O	HOH I 958	88.819	33.122	46.420	1.00	27.10		O
ANISOU40434	O	HOH I 958	3228	3067	3998	197	737	176	O
ATOM 40446	O	HOH I 962	61.700	24.339	37.540	1.00	29.91		O
ANISOU40446	O	HOH I 962	3676	3915	3774	-405	-201	-200	O
ATOM 40452	O	HOH I 964	79.036	10.825	50.418	1.00	32.30		O
ANISOU40452	O	HOH I 964	4456	3475	4341	283	-120	26	O
ATOM 40476	O	HOH I 972	66.603	18.545	39.877	0.00	28.19		O
ANISOU40476	O	HOH I 972	3635	3912	3165	287	234	75	O
ATOM 40635	O	HOH I1025	75.973	11.924	56.867	1.00	28.27		O
ANISOU40635	O	HOH I1025	3373	3496	3869	379	234	170	O
ATOM 40653	O	HOH I1031	86.010	13.779	51.750	1.00	37.18		O
ANISOU40653	O	HOH I1031	4682	4608	4833	59	109	65	O

ATOM 40767	O	HOH I1069	79.787	40.960	58.104	1.00	36.42		O
ANISOU40767	O	HOH I1069	4339	4769	4730	334	86	13	O
ATOM 40806	O	HOH I1082	84.999	17.603	52.422	1.00	27.50		O
ANISOU40806	O	HOH I1082	3243	3267	3937	-72	-17	139	O
ATOM 40833	O	HOH I1091	84.459	27.235	60.441	1.00	30.28		O
ANISOU40833	O	HOH I1091	3698	3634	4172	87	-74	289	O
ATOM 41034	O	HOH I1158	69.604	16.212	47.222	1.00	32.38		O
ANISOU41034	O	HOH I1158	4183	4264	3856	316	-32	-7	O
ATOM 41214	O	HOH I1218	70.544	29.378	40.838	1.00	34.08		O
ANISOU41214	O	HOH I1218	4076	4501	4370	-74	71	-38	O
ATOM 41307	O	HOH I1249	77.720	15.022	54.382	1.00	25.01		O
ANISOU41307	O	HOH I1249	3839	2205	3455	0	315	193	O
ATOM 41376	O	HOH I1272	92.164	29.566	60.811	1.00	41.16		O
ANISOU41376	O	HOH I1272	5062	5054	5520	4	187	-40	O
ATOM 41391	O	HOH I1277	78.225	35.244	37.422	1.00	45.50		O
ANISOU41391	O	HOH I1277	5680	5687	5920	-30	96	96	O
ATOM 41412	O	HOH I1284	62.209	24.973	34.838	1.00	49.83		O
ANISOU41412	O	HOH I1284	6142	6402	6390	9	3	-49	O
ATOM 41415	O	HOH I1285	78.559	31.939	37.407	1.00	35.91		O
ANISOU41415	O	HOH I1285	4282	4680	4680	-172	12	65	O
ATOM 41481	O	HOH I1307	83.630	23.857	43.928	1.00	39.19		O
ANISOU41481	O	HOH I1307	4814	5426	4650	149	60	100	O
ATOM 41529	O	HOH I1323	99.439	23.637	54.905	1.00	25.19		O
ANISOU41529	O	HOH I1323	3392	3000	3180	49	-4	173	O
ATOM 41613	O	HOH I1351	78.713	22.034	39.915	1.00	49.57		O
ANISOU41613	O	HOH I1351	6252	6307	6272	-17	77	-4	O
ATOM 41718	O	HOH I1386	78.105	20.078	42.022	1.00	38.92		O
ANISOU41718	O	HOH I1386	5107	4908	4771	-99	62	123	O
ATOM 41736	O	HOH I1392	83.573	16.260	46.747	1.00	39.58		O
ANISOU41736	O	HOH I1392	5199	4912	4926	92	-150	10	O
ATOM 41766	O	HOH I1402	65.274	25.273	36.276	1.00	30.66		O
ANISOU41766	O	HOH I1402	3979	4087	3582	-499	117	-181	O
ATOM 41775	O	HOH I1405	63.905	25.981	33.612	1.00	60.85		O
ANISOU41775	O	HOH I1405	7711	7766	7640	0	81	-2	O
ATOM 41865	O	HOH I1435	72.974	15.861	47.445	1.00	29.87		O
ANISOU41865	O	HOH I1435	4082	3226	4040	82	-147	-87	O
ATOM 41889	O	HOH I1443	88.700	26.970	34.611	1.00	46.25		O
ANISOU41889	O	HOH I1443	5763	5989	5822	-21	-12	13	O
ATOM 42012	O	HOH I1484	91.890	14.843	45.880	1.00	30.33		O
ANISOU42012	O	HOH I1484	3968	3237	4318	-203	100	-123	O
ATOM 42078	O	HOH I1506	64.224	14.605	43.908	1.00	39.80		O
ANISOU42078	O	HOH I1506	4983	5352	4785	-35	61	-96	O
ATOM 42186	O	HOH I1542	85.452	24.536	42.808	1.00	35.53		O
ANISOU42186	O	HOH I1542	4291	4665	4542	-383	-1	-16	O
ATOM 42393	O	HOH I1611	66.209	22.296	39.786	1.00	36.50		O
ANISOU42393	O	HOH I1611	4914	4434	4519	-37	109	-50	O
ATOM 42396	O	HOH I1612	67.389	15.483	40.662	1.00	51.12		O
ANISOU42396	O	HOH I1612	6740	6398	6284	-84	85	0	O
ATOM 42405	O	HOH I1615	92.896	23.214	35.963	1.00	46.09		O
ANISOU42405	O	HOH I1615	6086	5617	5808	-30	-73	-223	O
ATOM 42435	O	HOH I1625	86.422	25.216	40.369	1.00	46.61		O
ANISOU42435	O	HOH I1625	5836	5970	5900	-150	82	34	O
ATOM 42516	O	HOH I1652	68.375	14.168	47.274	1.00	27.12		O
ANISOU42516	O	HOH I1652	3886	3475	2942	382	42	366	O
ATOM 42783	O	HOH I1741	80.971	19.555	45.297	1.00	60.76		O
ANISOU42783	O	HOH I1741	7717	7577	7790	5	-10	12	O
ATOM 42831	O	HOH I1757	87.332	14.976	47.405	1.00	47.04		O
ANISOU42831	O	HOH I1757	5977	5977	5919	-43	-126	74	O
ATOM 42846	O	HOH I1762	76.590	10.990	52.768	1.00	44.72		O
ANISOU42846	O	HOH I1762	5801	5563	5625	-63	93	-23	O
ATOM 42882	O	HOH I1774	93.494	20.613	37.093	1.00	44.76		O

ANISOU42882	O	HOH I1774	5535	5819	5652	-165	94	23	O
ATOM 42969	O	HOH I1803	79.512	31.284	34.819	1.00	43.33		O
ANISOU42969	O	HOH I1803	5406	5557	5499	-7	-283	26	O
ATOM 43029	O	HOH I1823	74.883	17.439	45.078	1.00	49.34		O
ANISOU43029	O	HOH I1823	6136	6423	6186	82	-97	18	O
ATOM 43158	O	HOH I1866	82.139	27.856	33.595	1.00	29.87		O
ANISOU43158	O	HOH I1866	4055	3717	3576	-333	87	-286	O
ATOM 43293	O	HOH I1911	79.150	26.600	33.773	1.00	41.61		O
ANISOU43293	O	HOH I1911	5570	5292	4948	-109	-156	-29	O
ATOM 43305	O	HOH I1915	78.277	19.001	44.635	1.00	41.86		O
ANISOU43305	O	HOH I1915	5361	5267	5276	154	87	-104	O
ATOM 43422	O	HOH I1954	80.021	12.895	46.345	1.00	53.52		O
ANISOU43422	O	HOH I1954	6638	7049	6646	-63	128	68	O
ATOM 43554	O	HOH I1998	81.100	16.776	46.759	1.00	43.92		O
ANISOU43554	O	HOH I1998	5602	5605	5478	-61	138	-165	O
ATOM 43617	O	HOH I2019	91.203	22.559	37.690	1.00	48.97		O
ANISOU43617	O	HOH I2019	6251	6031	6322	31	64	-62	O
ATOM 43755	O	HOH I2065	66.142	18.386	34.319	1.00	48.98		O
ANISOU43755	O	HOH I2065	6185	6442	5982	6	-32	-23	O
ATOM 43836	O	HOH I2092	80.735	22.143	42.477	1.00	37.19		O
ANISOU43836	O	HOH I2092	4728	4763	4636	133	5	-182	O
ATOM 43875	O	HOH I2105	83.915	26.626	32.072	1.00	45.21		O
ANISOU43875	O	HOH I2105	5953	5465	5757	-117	165	-35	O
ATOM 43905	O	HOH I2115	83.540	25.970	35.651	1.00	46.05		O
ANISOU43905	O	HOH I2115	5968	5643	5884	50	-42	-133	O
ATOM 43956	O	HOH I2132	82.824	34.749	33.460	1.00	34.25		O
ANISOU43956	O	HOH I2132	4486	4435	4092	37	-105	-134	O
ATOM 43965	O	HOH I2135	68.875	13.908	44.337	1.00	53.45		O
ANISOU43965	O	HOH I2135	6754	6694	6859	-116	124	-141	O
ATOM 43983	O	HOH I2141	84.555	23.000	39.511	1.00	35.28		O
ANISOU43983	O	HOH I2141	3621	4916	4868	-159	195	156	O
ATOM 44025	O	HOH I2155	68.212	11.904	44.669	1.00	68.29		O
ANISOU44025	O	HOH I2155	8775	8627	8544	-34	36	-9	O
ATOM 44289	O	HOH I2243	70.303	18.163	43.625	1.00	44.02		O
ANISOU44289	O	HOH I2243	5768	5477	5481	32	3	-26	O
ATOM 44340	O	HOH I2260	77.299	11.249	43.900	1.00	62.73		O
ANISOU44340	O	HOH I2260	7898	8068	7869	-24	-7	14	O
ATOM 44352	O	HOH I2264	91.547	12.409	46.194	1.00	47.48		O
ANISOU44352	O	HOH I2264	6013	5720	6304	-85	-85	47	O
ATOM 44421	O	HOH I2287	66.076	22.939	34.318	1.00	47.34		O
ANISOU44421	O	HOH I2287	5956	6051	5978	-133	-17	-1	O
ATOM 44658	O	HOH I2366	92.333	40.065	50.189	1.00	40.05		O
ANISOU44658	O	HOH I2366	5206	4957	5051	-81	144	-124	O
ATOM 44781	O	HOH I2407	84.696	24.577	61.147	1.00	46.09		O
ANISOU44781	O	HOH I2407	5865	5622	6025	-2	-67	154	O
ATOM 45048	O	HOH I2496	71.587	15.143	43.827	1.00	42.91		O
ANISOU45048	O	HOH I2496	5416	5554	5332	9	-293	-85	O
ATOM 45087	O	HOH I2509	68.877	34.391	33.745	1.00	48.68		O
ANISOU45087	O	HOH I2509	6052	6308	6134	-79	-37	-51	O
ATOM 45126	O	HOH I2522	64.649	32.366	36.686	1.00	52.30		O
ANISOU45126	O	HOH I2522	6567	6707	6597	-33	-76	-45	O
ATOM 45300	O	HOH I2580	86.072	21.234	62.272	1.00	40.57		O
ANISOU45300	O	HOH I2580	4898	5267	5250	88	43	31	O
ATOM 45753	O	HOH I2731	64.365	21.736	33.031	1.00	40.46		O
ANISOU45753	O	HOH I2731	4897	5185	5289	-12	-20	17	O
ATOM 46146	O	HOH I2862	68.349	14.962	32.720	1.00	41.81		O
ANISOU46146	O	HOH I2862	5292	5631	4962	-79	11	-110	O
ATOM 46188	O	HOH I2876	85.649	15.223	40.779	1.00	62.78		O
ANISOU46188	O	HOH I2876	7864	7929	8058	4	-15	-74	O
ATOM 46293	O	HOH I2911	92.232	29.400	34.253	1.00	41.62		O
ANISOU46293	O	HOH I2911	4973	5606	5234	-145	33	-47	O

ATOM	46464	O	HOH I2968	85.429	20.036	51.002	1.00	25.74	O	
ANISOU	46464	O	HOH I2968	3335	2889	3554	-32	-69	-133	O
END										

Annex 1 Cont'd : 70

ACTIVE SITES

REMARK Created by MOLEMAN2 V. 990504/2.3 at Thu Jul 13 16:59:24 2000 for wulf

REMARK 3

REMARK 3 REFINEMENT.

REMARK 3 PROGRAM : REFMAC

REMARK 3 AUTHORS : MURSHUDOV, VAGIN, DODSON

REMARK 3

REMARK 3 Maximum likelihood refinement was used

REMARK 3

REMARK 3 DATA USED IN REFINEMENT.

REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.7

REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 73.

REMARK 3 DATA CUTOFF (SIGMA(F)) : 0.0

REMARK 3 COMPLETENESS FOR RANGE (%) : 82.7

REMARK 3 NUMBER OF REFLECTIONS : 230146

REMARK 3

REMARK 3 FIT TO DATA USED IN REFINEMENT.

REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT

REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM

REMARK 3 R VALUE (WORKING + TEST SET) : 0.16587

REMARK 3 R VALUE (WORKING SET) : 0.16312

REMARK 3 FREE R VALUE : 0.21818

REMARK 3 FREE R VALUE TEST SET SIZE (%) : 5.0

REMARK 3 FREE R VALUE TEST SET COUNT : 12192

REMARK 3

REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.

REMARK 3 All atoms : 46517

REMARK 3

REMARK 3 B VALUES.

REMARK 3 FROM WILSON PLOT (A**2) : NULL

REMARK 3 MEAN B VALUE (OVERALL, A**2) : 14.387

REMARK 3 OVERALL ANISOTROPIC B VALUE.

REMARK 3 B11 (A**2) : 0.46

REMARK 3 B22 (A**2) : -0.19

REMARK 3 B33 (A**2) : -0.27

REMARK 3 B12 (A**2) : 0.03

REMARK 3 B13 (A**2) : -0.02

REMARK 3 B23 (A**2) : -0.25

REMARK 3

REMARK 3 ESTIMATED OVERALL COORDINATE ERROR.

REMARK 3 ESU BASED ON R VALUE (A) :

REMARK 3 NULL

REMARK 3 ESU BASED ON FREE R VALUE (A) :

REMARK 3 0.18277

REMARK 3 ESU BASED ON MAXIMUM LIKELIHOOD (A) :

REMARK 3 0.12940

REMARK 3 ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2) :

REMARK 3 8.01924

REMARK 3

REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.

REMARK 3 DISTANCE RESTRAINTS. RMS SIGMA

REMARK 3 BOND LENGTH (A) : 0.021 ; 0.021

REMARK 3 BOND ANGLE (DEGREES) : 2.076 ; 2.015

REMARK 3 Torsion angles, period 1 (DEGREES) : 5.103 ; 3.000

REMARK 3 Torsion angles, period 3 (DEGREES) : 16.457 ; 15.000

REMARK 3 CHIRAL-CENTER RESTRAINTS (A**3) : 0.126 ; 0.200

REMARK 3 PLANE RESTRAINT (A) : 0.009 ; 0.020

REMARK 3 VDW repulsions (A) : 0.232 ; 0.300

REMARK 3 Potential hbonds (A) : 0.217 ; 0.500

REMARK 3

REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA

REMARK 3 MAIN-CHAIN BOND (A**2) : 1.443 ; 1.500

REMARK 3 MAIN-CHAIN ANGLE (A**2) : 2.158 ; 2.000
REMARK 3 SIDE-CHAIN BOND (A**2) : 3.125 ; 3.000
REMARK 3 SIDE-CHAIN ANGLE (A**2) : 4.584 ; 4.500
REMARK 3
REMARK 3 ANISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 Rigid-bond restraints (A**2) : 1.894 ; 2.000
REMARK 3 Sphericity; free atoms (A**2) : 4.664 ; 2.000
REMARK 3 Sphericity; bonded atoms (A**2) : 2.553 ; 2.000
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS.
REMARK 3
REMARK 3 TLS details
REMARK 3 Number of tls groups : 8
REMARK 3
REMARK 3 Number of pieces in the TLS group 1: 1
REMARK 3 From A 1 to A 292
REMARK 3 Origin for the group : 1
REMARK 3 69.4830 59.4220 78.9970
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0325 0.0433 0.0247 -0.0039 -0.0136 -0.0012
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6102 0.6435 0.4229 -0.1271 0.0884 -0.0867
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 0.0248 -0.0135 -0.0505 0.0232 0.0615 -0.0461 0.0207 -0.0758
REMARK 3
REMARK 3 Number of pieces in the TLS group 2: 1
REMARK 3 From B 1 to B 293
REMARK 3 Origin for the group : 2
REMARK 3 61.2650 33.4890 54.1360
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0294 0.0510 0.0183 0.0014 0.0082 -0.0045
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6794 0.6303 0.4419 0.1224 -0.1618 -0.1218
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0046 -0.0119 0.0109 0.0234 0.0528 0.0423 -0.0173 -0.0642
REMARK 3
REMARK 3 Number of pieces in the TLS group 3: 1
REMARK 3 From C 1 to C 292
REMARK 3 Origin for the group : 3
REMARK 3 100.4020 45.2900 79.2890
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0309 0.0357 0.0395 0.0126 0.0217 0.0172
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.5756 0.7497 0.6477 -0.1840 0.0581 -0.3103
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0999 -0.0112 0.0060 0.0283 -0.1071 -0.0800 0.0406 0.0887
REMARK 3
REMARK 3 Number of pieces in the TLS group 4: 1
REMARK 3 From D 1 to D 292
REMARK 3 Origin for the group : 4
REMARK 3 93.1810 38.1690 43.3930
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0110 0.0453 0.0536 0.0109 0.0225 0.0295
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6426 0.7184 0.8911 0.0882 -0.0950 -0.4089
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.1237 -0.0615 0.0018 -0.0411 -0.1339 -0.0574 0.0193 0.1369
REMARK 3
REMARK 3 Number of pieces in the TLS group 5: 1
REMARK 3 From E 1 to E 292
REMARK 3 Origin for the group : 5

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REMARK 3 42.8770 8.9030 19.5730
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0309 0.0452 0.0352 0.0089 -0.0125 -0.0200
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.6312 0.7631 0.9845 0.0814 0.0288 0.4970
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.1195 -0.0434 -0.0468 0.0342 0.1311 -0.0463 -0.0408 -0.1559
REMARK 3
REMARK 3 Number of pieces in the TLS group 6: 1
REMARK 3 From F 1 to F 293
REMARK 3 Origin for the group : 6
REMARK 3 38.0920 17.7800 -16.3490
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0208 0.0425 0.0417 0.0034 0.0045 -0.0015
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.8800 0.3582 0.6933 0.1180 0.1354 0.1904
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0810 0.0464 -0.0329 0.0291 0.0416 0.0160 -0.0440 -0.0740
REMARK 3
REMARK 3 Number of pieces in the TLS group 7: 1
REMARK 3 From G 1 to G 292
REMARK 3 Origin for the group : 7
REMARK 3 71.8950 21.8640 -15.9250
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0234 0.0522 0.0272 -0.0024 -0.0109 0.0094
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.5696 0.5742 0.4250 0.0699 -0.0286 -0.0019
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0333 0.0146 0.0152 -0.0110 -0.0283 0.0204 -0.0007 0.0589
REMARK 3
REMARK 3 Number of pieces in the TLS group 8: 1
REMARK 3 From H 1 to H 292
REMARK 3 Origin for the group : 8
REMARK 3 71.9070 -5.2410 8.8240
REMARK 3 T tensor (T11, T22, T33, T12, T13, T23)
REMARK 3 0.0445 0.0386 0.0064 0.0038 0.0132 0.0109
REMARK 3 L tensor (L11, L22, L33, L12, L13, L23)
REMARK 3 0.4837 0.7743 0.6523 -0.1036 -0.1161 0.0699
REMARK 3 S tensor (S22-S11, S11-S33, S12, S13, S23, S21, S31)
REMARK 3 -0.0109 -0.0288 -0.0166 0.0049 -0.0575 -0.0486 0.0096 0.0981
REMARK 3
REMARK 3 Hydrogens have been added in the riding positions
REMARK 3
REMARK 3
REMARK 3 Scaling details
REMARK 3 Babinet"s principle for scaling has been used
REMARK 3 Bulk solvent correction based on constant value has been used
REMARK 3 Parameters for mask calculation
REMARK 3 VDW prob radii = 1.40
REMARK 3 ION prob radii = 0.80
REMARK 3 Shrinkage radii = 0.80
REMARK 3
HEADER ---- XX-XXX-XX xxxx
COMPND ---
CISPEP 1 HIS A 16 PRO A 17 0.00
CISPEP 2 HIS B 17 PRO B 18 0.00
CISPEP 3 HIS C 16 PRO C 17 0.00
CISPEP 4 HIS D 16 PRO D 17 0.00
CISPEP 5 HIS E 16 PRO E 17 0.00
CISPEP 6 HIS G 16 PRO G 17 0.00
CISPEP 7 HIS H 16 PRO H 17 0.00

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CISPEP	8	HIS	F	17	PRO	F	18	0.00				
CRYST1	71.575	73.410	134.290	89.94	80.61	80.93	P 1	1				
ORIGX1	1.000000	0.000000	0.000000			0.000000						
ORIGX2	0.000000	1.000000	0.000000			0.000000						
ORIGX3	0.000000	0.000000	1.000000			0.000000						
SCALE1	0.013971	-0.002230	-0.002368			0.000000						
SCALE2	0.000000	0.013795	0.000349			0.000000						
SCALE3	0.000000	0.000000	0.007550			0.000000						
ATOM	328	CD1	ILE	A	22	59.967	47.366	65.615	1.00	33.85		C
ANISOU	328	CD1	ILE	A	22	4267	4278	4314	26	53	-50	C
ATOM	432	CG	PRO	A	28	66.308	45.162	69.043	1.00	13.58		C
ANISOU	432	CG	PRO	A	28	1807	1645	1708	59	-94	-91	C
ATOM	4272	N	LYS	A	276	63.617	31.206	81.166	1.00	20.93		N
ANISOU	4272	N	LYS	A	276	2678	2673	2601	-66	43	-61	N
ATOM	4274	CA	LYS	A	276	63.911	30.276	80.088	1.00	22.01		C
ANISOU	4274	CA	LYS	A	276	2776	2842	2744	-36	48	-29	C
ATOM	4276	CB	LYS	A	276	62.666	29.928	79.262	1.00	22.43		C
ANISOU	4276	CB	LYS	A	276	2800	2903	2817	-15	-31	-11	C
ATOM	4279	CG	LYS	A	276	61.548	29.173	80.028	1.00	24.80		C
ANISOU	4279	CG	LYS	A	276	3078	3271	3071	-51	104	-9	C
ATOM	4282	CD	LYS	A	276	61.850	27.689	80.289	1.00	28.12		C
ANISOU	4282	CD	LYS	A	276	3580	3521	3582	-14	38	85	C
ATOM	4285	CE	LYS	A	276	61.479	26.778	79.084	1.00	30.97		C
ANISOU	4285	CE	LYS	A	276	4025	3975	3765	-22	-7	-28	C
ATOM	4288	NZ	LYS	A	276	61.473	25.294	79.348	1.00	33.41		N
ANISOU	4288	NZ	LYS	A	276	4357	4145	4192	-1	0	31	N
ATOM	4292	C	LYS	A	276	64.962	30.874	79.183	1.00	21.47		C
ANISOU	4292	C	LYS	A	276	2695	2761	2698	-38	27	-49	C
ATOM	4293	O	LYS	A	276	65.346	30.254	78.213	1.00	21.93		O
ANISOU	4293	O	LYS	A	276	2808	2846	2675	-109	-37	-263	O
ATOM	4294	N	ASN	A	277	65.439	32.067	79.497	1.00	20.65		N
ANISOU	4294	N	ASN	A	277	2652	2640	2551	6	-13	-71	N
ATOM	4296	CA	ASN	A	277	66.438	32.690	78.652	1.00	19.73		C
ANISOU	4296	CA	ASN	A	277	2515	2478	2503	-15	-15	-54	C
ATOM	4298	CB	ASN	A	277	65.754	33.728	77.777	1.00	20.79		C
ANISOU	4298	CB	ASN	A	277	2641	2661	2597	4	-33	-11	C
ATOM	4301	CG	ASN	A	277	64.999	34.796	78.617	1.00	22.82		C
ANISOU	4301	CG	ASN	A	277	2899	2803	2968	-5	-62	-172	C
ATOM	4302	OD1	ASN	A	277	65.656	35.665	79.160	1.00	20.73		O
ANISOU	4302	OD1	ASN	A	277	2630	2112	3134	-213	-58	282	O
ATOM	4303	ND2	ASN	A	277	63.604	34.677	78.777	1.00	23.06		N
ANISOU	4303	ND2	ASN	A	277	2877	3050	2833	-178	34	-47	N
ATOM	4306	C	ASN	A	277	67.629	33.274	79.432	1.00	19.02		C
ANISOU	4306	C	ASN	A	277	2493	2406	2327	57	7	-31	C
ATOM	4308	N	GLY	A	278	68.634	33.764	78.693	1.00	16.96		N
ANISOU	4308	N	GLY	A	278	2237	2114	2091	-42	-46	-54	N
ATOM	4654	CA	GLY	B	5	53.052	32.510	49.620	1.00	8.62		C
ANISOU	4654	CA	GLY	B	5	1034	1119	1121	131	38	18	C
ATOM	4657	C	GLY	B	5	52.521	32.740	51.044	1.00	8.23		C
ANISOU	4657	C	GLY	B	5	1027	1023	1078	21	-26	-110	C
ATOM	4658	O	GLY	B	5	51.452	33.330	51.223	1.00	7.96		O
ANISOU	4658	O	GLY	B	5	861	1053	1109	99	-52	-212	O
ATOM	4659	N	ILE	B	6	53.253	32.209	52.017	1.00	7.06		N
ANISOU	4659	N	ILE	B	6	713	943	1026	57	58	-14	N
ATOM	4661	CA	ILE	B	6	53.005	32.398	53.422	1.00	7.81		C
ANISOU	4661	CA	ILE	B	6	893	1031	1042	62	-58	-29	C
ATOM	4663	CB	ILE	B	6	52.441	31.143	54.056	1.00	7.78		C
ANISOU	4663	CB	ILE	B	6	920	1034	1000	102	-106	-1	C
ATOM	4665	CG1	ILE	B	6	51.270	30.624	53.275	1.00	10.95		C
ANISOU	4665	CG1	ILE	B	6	1124	1370	1665	-16	-74	-78	C
ATOM	4668	CD1	ILE	B	6	50.634	29.447	53.966	1.00	11.37		C

ANISOU	4668	CD1	ILE	B	6	1342	1616	1360	-189	-124	98	C
ATOM	4672	CG2	ILE	B	6	52.085	31.412	55.516	1.00	8.38		C
ANISOU	4672	CG2	ILE	B	6	966	1112	1106	36	-72	121	C
ATOM	4676	C	ILE	B	6	54.268	32.714	54.166	1.00	7.81		C
ANISOU	4676	C	ILE	B	6	872	1070	1023	17	39	66	C
ATOM	4677	O	ILE	B	6	55.322	32.027	53.970	1.00	9.13		O
ANISOU	4677	O	ILE	B	6	877	1163	1430	180	-200	39	O
ATOM	4678	N	ILE	B	7	54.186	33.767	54.973	1.00	8.62		N
ANISOU	4678	N	ILE	B	7	867	1194	1213	149	-99	30	N
ATOM	4680	CA	ILE	B	7	55.273	34.105	55.910	1.00	9.24		C
ANISOU	4680	CA	ILE	B	7	1136	1235	1137	41	-23	14	C
ATOM	4682	CB	ILE	B	7	55.694	35.537	55.868	1.00	10.30		C
ANISOU	4682	CB	ILE	B	7	1301	1421	1190	-18	-22	-15	C
ATOM	4684	CG1	ILE	B	7	56.111	35.974	54.453	1.00	10.33		C
ANISOU	4684	CG1	ILE	B	7	1317	1288	1319	93	210	102	C
ATOM	4687	CD1	ILE	B	7	56.320	37.425	54.375	1.00	10.11		C
ANISOU	4687	CD1	ILE	B	7	1084	1503	1253	-195	311	117	C
ATOM	4691	CG2	ILE	B	7	56.887	35.764	56.869	1.00	9.63		C
ANISOU	4691	CG2	ILE	B	7	1070	1233	1356	80	-151	-68	C
ATOM	4695	C	ILE	B	7	54.804	33.759	57.296	1.00	8.87		C
ANISOU	4695	C	ILE	B	7	1024	1198	1147	20	45	-4	C
ATOM	4696	O	ILE	B	7	53.848	34.341	57.766	1.00	7.45		O
ANISOU	4696	O	ILE	B	7	488	1146	1196	-11	50	146	O
ATOM	4697	N	LEU	B	8	55.547	32.872	57.988	1.00	8.33		N
ANISOU	4697	N	LEU	B	8	911	1085	1168	68	67	36	N
ATOM	4699	CA	LEU	B	8	55.220	32.551	59.377	1.00	8.71		C
ANISOU	4699	CA	LEU	B	8	886	1279	1145	1	15	17	C
ATOM	4701	CB	LEU	B	8	55.444	31.085	59.673	1.00	8.42		C
ANISOU	4701	CB	LEU	B	8	848	1164	1186	83	12	-61	C
ATOM	4704	CG	LEU	B	8	54.937	30.427	60.947	1.00	13.63		C
ANISOU	4704	CG	LEU	B	8	1659	1822	1697	42	33	-9	C
ATOM	4706	CD1	LEU	B	8	53.455	30.654	61.157	1.00	13.18		C
ANISOU	4706	CD1	LEU	B	8	1440	1872	1693	17	67	134	C
ATOM	4710	CD2	LEU	B	8	55.189	28.950	61.003	1.00	14.77		C
ANISOU	4710	CD2	LEU	B	8	1701	1898	2011	197	-83	33	C
ATOM	4714	C	LEU	B	8	56.066	33.473	60.246	1.00	8.77		C
ANISOU	4714	C	LEU	B	8	1016	1241	1073	9	19	117	C
ATOM	4715	O	LEU	B	8	57.309	33.329	60.288	1.00	8.90		O
ANISOU	4715	O	LEU	B	8	772	1585	1022	-62	-80	134	O
ATOM	4716	N	ALA	B	9	55.418	34.470	60.831	1.00	9.86		N
ANISOU	4716	N	ALA	B	9	989	1477	1279	-44	84	24	N
ATOM	4718	CA	ALA	B	9	56.095	35.542	61.548	1.00	10.37		C
ANISOU	4718	CA	ALA	B	9	1209	1347	1384	47	12	-2	C
ATOM	4720	CB	ALA	B	9	55.998	36.760	60.777	1.00	11.75		C
ANISOU	4720	CB	ALA	B	9	1343	1553	1569	51	-52	-55	C
ATOM	4724	C	ALA	B	9	55.607	35.757	62.965	1.00	11.00		C
ANISOU	4724	C	ALA	B	9	1263	1421	1494	43	-9	-34	C
ATOM	4725	O	ALA	B	9	55.473	36.905	63.428	1.00	11.38		O
ANISOU	4725	O	ALA	B	9	1194	1494	1636	-105	-33	-67	O
ATOM	4726	N	GLY	B	10	55.253	34.650	63.604	1.00	11.58		N
ANISOU	4726	N	GLY	B	10	1334	1459	1606	-26	-27	-33	N
ATOM	4728	CA	GLY	B	10	54.806	34.643	64.955	1.00	12.14		C
ANISOU	4728	CA	GLY	B	10	1404	1614	1594	-11	-36	-9	C
ATOM	4731	C	GLY	B	10	55.867	34.159	65.918	1.00	13.80		C
ANISOU	4731	C	GLY	B	10	1615	1866	1759	-55	-98	9	C
ATOM	4732	O	GLY	B	10	57.042	34.470	65.782	1.00	10.83		O
ANISOU	4732	O	GLY	B	10	1024	1785	1305	91	-348	-50	O
ATOM	4733	N	GLY	B	11	55.441	33.393	66.902	1.00	15.86		N
ANISOU	4733	N	GLY	B	11	1891	2141	1993	-145	-64	98	N
ATOM	4735	CA	GLY	B	11	56.356	32.896	67.932	1.00	18.72		C
ANISOU	4735	CA	GLY	B	11	2268	2394	2451	-69	-72	89	C

ATOM	4738	C	GLY	B	11	56.583	33.905	69.053	1.00	21.22		C
ANISOU	4738	C	GLY	B	11	2691	2766	2602	5	-29	-24	C
ATOM	4739	O	GLY	B	11	56.307	35.125	68.902	1.00	21.22		O
ANISOU	4739	O	GLY	B	11	2619	2925	2517	37	-175	-28	O
ATOM	4740	N	SER	B	12	57.164	33.401	70.145	1.00	24.10		N
ANISOU	4740	N	SER	B	12	3060	3108	2988	66	-56	31	N
ATOM	4742	CA	SER	B	12	57.398	34.142	71.396	1.00	25.99		C
ANISOU	4742	CA	SER	B	12	3317	3290	3268	53	-70	7	C
ATOM	4744	CB	SER	B	12	57.390	33.084	72.522	1.00	27.20		C
ANISOU	4744	CB	SER	B	12	3513	3488	3331	34	34	26	C
ATOM	4747	OG	SER	B	12	58.313	32.017	72.217	1.00	31.02		O
ANISOU	4747	OG	SER	B	12	3951	3661	4174	130	-145	-14	O
ATOM	4749	C	SER	B	12	58.711	34.979	71.435	1.00	26.05		C
ANISOU	4749	C	SER	B	12	3296	3334	3265	74	-62	-16	C
ATOM	4750	O	SER	B	12	58.847	35.965	72.200	1.00	27.75		O
ANISOU	4750	O	SER	B	12	3451	3458	3631	109	-142	53	O
ATOM	4751	N	GLY	B	13	59.695	34.585	70.640	1.00	25.18		N
ANISOU	4751	N	GLY	B	13	3171	3282	3114	31	-100	18	N
ATOM	4753	CA	GLY	B	13	60.978	35.257	70.614	1.00	24.90		C
ANISOU	4753	CA	GLY	B	13	3228	3139	3092	-17	-53	4	C
ATOM	4756	C	GLY	B	13	61.702	35.190	71.959	1.00	24.18		C
ANISOU	4756	C	GLY	B	13	3041	3069	3077	14	-79	36	C
ATOM	4757	O	GLY	B	13	62.504	36.091	72.293	1.00	24.09		O
ANISOU	4757	O	GLY	B	13	3096	2846	3208	-12	-13	99	O
ATOM	4758	N	THR	B	14	61.418	34.155	72.747	1.00	23.43		N
ANISOU	4758	N	THR	B	14	2934	2945	3024	-75	-73	-14	N
ATOM	4760	CA	THR	B	14	62.039	33.999	74.095	1.00	23.26		C
ANISOU	4760	CA	THR	B	14	2917	2923	2997	-2	-47	10	C
ATOM	4762	CB	THR	B	14	61.656	32.636	74.640	1.00	23.77		C
ANISOU	4762	CB	THR	B	14	2909	3078	3042	-31	24	30	C
ATOM	4764	OG1	THR	B	14	60.232	32.596	74.876	1.00	25.47		O
ANISOU	4764	OG1	THR	B	14	2930	3108	3640	71	-29	49	O
ATOM	4766	CG2	THR	B	14	62.232	32.400	75.994	1.00	24.62		C
ANISOU	4766	CG2	THR	B	14	3048	3159	3147	-45	7	46	C
ATOM	4770	C	THR	B	14	63.573	34.206	74.114	1.00	23.18		C
ANISOU	4770	C	THR	B	14	2944	2938	2924	-11	-8	-4	C
ATOM	4771	O	THR	B	14	64.134	34.980	74.942	1.00	22.98		O
ANISOU	4771	O	THR	B	14	2877	2886	2968	-24	-38	-97	O
ATOM	4772	N	ARG	B	15	64.293	33.558	73.220	1.00	22.84		N
ANISOU	4772	N	ARG	B	15	2926	2824	2926	4	-36	-58	N
ATOM	4774	CA	ARG	B	15	65.765	33.741	73.237	1.00	23.13		C
ANISOU	4774	CA	ARG	B	15	2934	2881	2971	-18	-23	-18	C
ATOM	4776	CB	ARG	B	15	66.438	32.910	72.162	1.00	24.19		C
ANISOU	4776	CB	ARG	B	15	3004	3059	3125	3	-20	-71	C
ATOM	4779	CG	ARG	B	15	66.233	31.423	72.405	1.00	26.14		C
ANISOU	4779	CG	ARG	B	15	3334	3177	3418	-5	-8	66	C
ATOM	4782	CD	ARG	B	15	66.636	30.526	71.228	1.00	30.66		C
ANISOU	4782	CD	ARG	B	15	3916	3876	3855	71	80	-99	C
ATOM	4785	NE	ARG	B	15	65.682	30.594	70.127	1.00	33.05		N
ANISOU	4785	NE	ARG	B	15	4150	4267	4139	36	23	-43	N
ATOM	4787	CZ	ARG	B	15	65.992	30.490	68.841	1.00	34.85		C
ANISOU	4787	CZ	ARG	B	15	4461	4409	4372	-28	12	3	C
ATOM	4788	NH1	ARG	B	15	67.267	30.299	68.467	1.00	36.37		N
ANISOU	4788	NH1	ARG	B	15	4506	4533	4777	-35	108	25	N
ATOM	4791	NH2	ARG	B	15	65.028	30.565	67.928	1.00	33.50		N
ANISOU	4791	NH2	ARG	B	15	4310	4098	4318	-57	-27	21	N
ATOM	4794	C	ARG	B	15	66.232	35.222	73.153	1.00	22.53		C
ANISOU	4794	C	ARG	B	15	2842	2821	2895	1	-14	-23	C
ATOM	4795	O	ARG	B	15	67.323	35.575	73.649	1.00	21.79		O
ANISOU	4795	O	ARG	B	15	2737	2767	2773	-37	52	-36	O
ATOM	4796	N	LEU	B	16	65.387	36.088	72.591	1.00	21.89		N

ANISOU	4796	N	LEU	B	16	2815	2704	2799	-71	-78	-12	N
ATOM	4798	CA	LEU	B	16	65.751	37.502	72.466	1.00	21.56		C
ANISOU	4798	CA	LEU	B	16	2763	2676	2750	13	-63	37	C
ATOM	4800	CB	LEU	B	16	65.338	38.016	71.098	1.00	20.99		C
ANISOU	4800	CB	LEU	B	16	2564	2721	2688	21	-56	13	C
ATOM	4803	CG	LEU	B	16	66.028	37.289	69.966	1.00	22.08		C
ANISOU	4803	CG	LEU	B	16	2675	2893	2821	10	-39	-8	C
ATOM	4805	CD1	LEU	B	16	65.480	37.772	68.657	1.00	23.18		C
ANISOU	4805	CD1	LEU	B	16	2789	3105	2913	102	7	13	C
ATOM	4809	CD2	LEU	B	16	67.595	37.513	70.012	1.00	23.46		C
ANISOU	4809	CD2	LEU	B	16	2847	3058	3009	-3	-22	-99	C
ATOM	4813	C	LEU	B	16	65.280	38.427	73.615	1.00	20.96		C
ANISOU	4813	C	LEU	B	16	2692	2590	2680	6	-69	57	C
ATOM	4814	O	LEU	B	16	65.574	39.653	73.604	1.00	21.14		O
ANISOU	4814	O	LEU	B	16	2957	2456	2617	-27	-152	193	O
ATOM	4815	N	HIS	B	17	64.642	37.855	74.637	1.00	19.82		N
ANISOU	4815	N	HIS	B	17	2560	2374	2595	-38	-56	46	N
ATOM	4817	CA	HIS	B	17	64.185	38.633	75.776	1.00	19.95		C
ANISOU	4817	CA	HIS	B	17	2511	2435	2634	-17	-62	41	C
ATOM	4819	CB	HIS	B	17	63.594	37.771	76.888	1.00	20.09		C
ANISOU	4819	CB	HIS	B	17	2595	2471	2567	6	-52	77	C
ATOM	4822	CG	HIS	B	17	62.173	37.362	76.665	1.00	23.15		C
ANISOU	4822	CG	HIS	B	17	2775	2962	3057	-25	-61	67	C
ATOM	4823	ND1	HIS	B	17	61.442	37.780	75.575	1.00	25.02		N
ANISOU	4823	ND1	HIS	B	17	3252	3089	3165	8	-94	159	N
ATOM	4825	CE1	HIS	B	17	60.188	37.387	75.734	1.00	25.92		C
ANISOU	4825	CE1	HIS	B	17	3188	3272	3389	-107	-54	114	C
ATOM	4827	NE2	HIS	B	17	60.159	36.496	76.714	1.00	25.98		N
ANISOU	4827	NE2	HIS	B	17	3136	3367	3366	-140	-49	57	N
ATOM	4829	CD2	HIS	B	17	61.409	36.421	77.279	1.00	24.62		C
ANISOU	4829	CD2	HIS	B	17	3150	3052	3152	-65	-86	171	C
ATOM	4831	C	HIS	B	17	65.412	39.382	76.317	1.00	18.59		C
ANISOU	4831	C	HIS	B	17	2344	2255	2462	-8	-74	0	C
ATOM	4832	O	HIS	B	17	66.510	38.835	76.288	1.00	18.10		O
ANISOU	4832	O	HIS	B	17	2242	2080	2556	-107	-58	95	O
ATOM	4851	CB	ALA	B	19	65.466	42.826	72.576	1.00	14.83		C
ANISOU	4851	CB	ALA	B	19	1813	1767	2053	-157	-35	-55	C
ATOM	4855	C	ALA	B	19	62.942	42.771	72.870	1.00	16.33		C
ANISOU	4855	C	ALA	B	19	1931	2057	2215	-59	-79	62	C
ATOM	4856	O	ALA	B	19	62.233	43.673	72.438	1.00	16.77		O
ANISOU	4856	O	ALA	B	19	2027	1865	2480	-38	-88	4	O
ATOM	4857	N	THR	B	20	62.568	41.500	72.794	1.00	16.98		N
ANISOU	4857	N	THR	B	20	2123	2072	2254	-20	-143	-22	N
ATOM	4859	CA	THR	B	20	61.257	41.119	72.214	1.00	18.21		C
ANISOU	4859	CA	THR	B	20	2239	2345	2335	-35	-27	-16	C
ATOM	4861	CB	THR	B	20	61.314	39.725	71.669	1.00	17.86		C
ANISOU	4861	CB	THR	B	20	2209	2279	2298	-91	-7	2	C
ATOM	4863	OG1	THR	B	20	61.904	38.854	72.642	1.00	17.92		O
ANISOU	4863	OG1	THR	B	20	2537	2073	2197	-122	-174	-51	O
ATOM	4865	CG2	THR	B	20	62.332	39.676	70.526	1.00	18.52		C
ANISOU	4865	CG2	THR	B	20	2465	2331	2237	-110	122	-75	C
ATOM	4869	C	THR	B	20	60.072	41.247	73.155	1.00	19.59		C
ANISOU	4869	C	THR	B	20	2367	2545	2529	-34	-31	-9	C
ATOM	4870	O	THR	B	20	59.005	40.734	72.852	1.00	18.68		O
ANISOU	4870	O	THR	B	20	1946	2752	2397	-81	-23	-90	O
ATOM	4871	N	LEU	B	21	60.262	41.859	74.313	1.00	20.51		N
ANISOU	4871	N	LEU	B	21	2600	2632	2561	-11	-85	-72	N
ATOM	4873	CA	LEU	B	21	59.119	42.158	75.148	1.00	22.04		C
ANISOU	4873	CA	LEU	B	21	2713	2848	2811	-30	7	-18	C
ATOM	4900	N	ILE	B	23	58.881	44.356	71.035	1.00	28.39		N
ANISOU	4900	N	ILE	B	23	3571	3632	3581	78	-25	-57	N

ATOM	4902	CA	ILE	B	23	58.468	44.083	69.655	1.00	28.26		C
ANISOU	4902	CA	ILE	B	23	3667	3572	3495	48	-45	-51	C
ATOM	4904	CB	ILE	B	23	59.491	44.850	68.829	1.00	29.70		C
ANISOU	4904	CB	ILE	B	23	3806	3766	3709	-4	-55	-30	C
ATOM	4906	CG1	ILE	B	23	59.480	46.331	69.174	1.00	33.33		C
ANISOU	4906	CG1	ILE	B	23	4333	4116	4215	5	-28	20	C
ATOM	4913	CG2	ILE	B	23	59.309	44.662	67.361	1.00	31.12		C
ANISOU	4913	CG2	ILE	B	23	3979	4049	3796	4	-34	46	C
ATOM	4917	C	ILE	B	23	58.573	42.583	69.222	1.00	26.14		C
ANISOU	4917	C	ILE	B	23	3361	3354	3217	83	-102	-65	C
ATOM	4918	O	ILE	B	23	59.412	41.878	69.764	1.00	26.46		O
ANISOU	4918	O	ILE	B	23	3613	3384	3054	167	-200	-74	O
ATOM	4919	N	SER	B	24	57.781	42.124	68.223	1.00	22.94		N
ANISOU	4919	N	SER	B	24	2867	2910	2936	146	-21	-55	N
ATOM	4921	CA	SER	B	24	57.934	40.781	67.625	1.00	20.06		C
ANISOU	4921	CA	SER	B	24	2483	2665	2472	1	-27	20	C
ATOM	4923	CB	SER	B	24	56.993	40.556	66.420	1.00	20.18		C
ANISOU	4923	CB	SER	B	24	2475	2606	2586	-27	29	14	C
ATOM	4926	OG	SER	B	24	57.316	39.383	65.641	1.00	19.44		O
ANISOU	4926	OG	SER	B	24	2256	2513	2616	210	85	116	O
ATOM	4928	C	SER	B	24	59.353	40.734	67.107	1.00	17.16		C
ANISOU	4928	C	SER	B	24	2132	2321	2066	8	-77	-46	C
ATOM	4929	O	SER	B	24	59.856	41.739	66.618	1.00	15.55		O
ANISOU	4929	O	SER	B	24	1769	2319	1818	57	-130	-193	O
ATOM	4930	N	LYS	B	25	59.961	39.565	67.149	1.00	15.63		N
ANISOU	4930	N	LYS	B	25	1859	2224	1854	-23	-54	-12	N
ATOM	4932	CA	LYS	B	25	61.286	39.394	66.574	1.00	17.41		C
ANISOU	4932	CA	LYS	B	25	2097	2301	2217	-35	-81	4	C
ATOM	4934	CB	LYS	B	25	61.691	37.890	66.723	1.00	18.55		C
ANISOU	4934	CB	LYS	B	25	2268	2376	2404	33	-62	-31	C
ATOM	4937	CG	LYS	B	25	62.903	37.414	65.898	1.00	21.45		C
ANISOU	4937	CG	LYS	B	25	2599	2829	2721	-54	73	-5	C
ATOM	4940	CD	LYS	B	25	63.429	36.045	66.323	1.00	24.70		C
ANISOU	4940	CD	LYS	B	25	2955	3220	3209	37	-12	86	C
ATOM	4943	CE	LYS	B	25	62.583	34.836	66.028	1.00	26.45		C
ANISOU	4943	CE	LYS	B	25	3461	3257	3330	55	-43	-81	C
ATOM	4946	NZ	LYS	B	25	63.244	33.631	66.721	1.00	27.46		N
ANISOU	4946	NZ	LYS	B	25	3550	3408	3476	9	-60	73	N
ATOM	4950	C	LYS	B	25	61.277	39.851	65.103	1.00	16.13		C
ANISOU	4950	C	LYS	B	25	1859	2213	2053	-65	-62	43	C
ATOM	4951	O	LYS	B	25	62.225	40.491	64.603	1.00	17.01		O
ANISOU	4951	O	LYS	B	25	1786	2328	2348	-117	-286	12	O
ATOM	4952	N	GLN	B	26	60.172	39.607	64.393	1.00	14.29		N
ANISOU	4952	N	GLN	B	26	1683	1850	1895	-99	-30	-42	N
ATOM	4954	CA	GLN	B	26	60.135	39.935	62.967	1.00	12.33		C
ANISOU	4954	CA	GLN	B	26	1412	1627	1645	-3	-2	-68	C
ATOM	4956	CB	GLN	B	26	59.160	38.991	62.227	1.00	13.77		C
ANISOU	4956	CB	GLN	B	26	1582	1815	1835	-54	-67	31	C
ATOM	4959	CG	GLN	B	26	59.617	37.546	62.067	1.00	11.76		C
ANISOU	4959	CG	GLN	B	26	1005	1916	1545	-26	334	-281	C
ATOM	4962	CD	GLN	B	26	59.581	36.689	63.315	1.00	16.15		C
ANISOU	4962	CD	GLN	B	26	2046	2170	1919	-41	-107	-222	C
ATOM	4963	OE1	GLN	B	26	60.566	36.008	63.615	1.00	22.97		O
ANISOU	4963	OE1	GLN	B	26	2888	2905	2932	273	-104	-351	O
ATOM	4964	NE2	GLN	B	26	58.478	36.710	64.051	1.00	14.40		N
ANISOU	4964	NE2	GLN	B	26	1690	2101	1678	-270	-82	-253	N
ATOM	4967	C	GLN	B	26	59.904	41.406	62.600	1.00	12.55		C
ANISOU	4967	C	GLN	B	26	1336	1821	1610	-28	-28	-8	C
ATOM	4968	O	GLN	B	26	59.895	41.750	61.446	1.00	10.35		O
ANISOU	4968	O	GLN	B	26	820	1519	1593	55	8	144	O
ATOM	4969	N	LEU	B	27	59.665	42.252	63.599	1.00	12.42		N

ANISOU	4969	N	LEU	B	27	1476	1594	1645	73	-87	-57	N
ATOM	4971	CA	LEU	B	27	59.570	43.668	63.386	1.00	14.13		C
ANISOU	4971	CA	LEU	B	27	1761	1870	1737	-8	-24	-33	C
ATOM	4973	CB	LEU	B	27	58.417	44.261	64.210	1.00	14.30		C
ANISOU	4973	CB	LEU	B	27	1728	1828	1878	53	2	61	C
ATOM	4976	CG	LEU	B	27	56.953	43.908	63.857	1.00	17.96		C
ANISOU	4976	CG	LEU	B	27	2258	2430	2135	-119	-90	-45	C
ATOM	4978	CD1	LEU	B	27	55.985	44.028	65.028	1.00	19.08		C
ANISOU	4978	CD1	LEU	B	27	2174	2447	2626	122	78	-26	C
ATOM	4982	CD2	LEU	B	27	56.513	44.848	62.793	1.00	22.11		C
ANISOU	4982	CD2	LEU	B	27	2759	2721	2921	2	-188	170	C
ATOM	4986	C	LEU	B	27	60.891	44.309	63.775	1.00	14.03		C
ANISOU	4986	C	LEU	B	27	1766	1801	1763	1	55	-12	C
ATOM	4987	O	LEU	B	27	61.067	45.442	63.475	1.00	17.04		O
ANISOU	4987	O	LEU	B	27	2240	2003	2228	-14	-5	-49	O
ATOM	4988	N	LEU	B	28	61.835	43.599	64.409	1.00	14.02		N
ANISOU	4988	N	LEU	B	28	1660	1909	1756	-90	22	13	N
ATOM	4990	CA	LEU	B	28	63.150	44.224	64.778	1.00	13.99		C
ANISOU	4990	CA	LEU	B	28	1700	1844	1770	-48	28	-6	C
ATOM	4992	CB	LEU	B	28	63.975	43.297	65.652	1.00	14.06		C
ANISOU	4992	CB	LEU	B	28	1569	1932	1840	-71	-4	28	C
ATOM	4995	CG	LEU	B	28	63.284	42.777	66.926	1.00	16.82		C
ANISOU	4995	CG	LEU	B	28	2083	2235	2070	-22	15	-12	C
ATOM	4997	CD1	LEU	B	28	64.143	41.766	67.650	1.00	17.68		C
ANISOU	4997	CD1	LEU	B	28	2269	2266	2183	29	-66	-47	C
ATOM	5001	CD2	LEU	B	28	62.938	43.956	67.787	1.00	17.08		C
ANISOU	5001	CD2	LEU	B	28	2064	2215	2209	-97	30	-130	C
ATOM	5005	C	LEU	B	28	63.959	44.497	63.522	1.00	12.02		C
ANISOU	5005	C	LEU	B	28	1390	1585	1593	-9	-12	-1	C
ATOM	5006	O	LEU	B	28	63.867	43.764	62.571	1.00	11.97		O
ANISOU	5006	O	LEU	B	28	1322	1608	1617	-216	-266	-58	O
ATOM	5007	N	PRO	B	29	64.797	45.511	63.514	1.00	11.04		N
ANISOU	5007	N	PRO	B	29	1405	1409	1380	-60	-6	-23	N
ATOM	5008	CA	PRO	B	29	65.582	45.786	62.322	1.00	10.79		C
ANISOU	5008	CA	PRO	B	29	1354	1313	1432	-38	40	-46	C
ATOM	5016	CD	PRO	B	29	65.040	46.471	64.594	1.00	12.34		C
ANISOU	5016	CD	PRO	B	29	1490	1521	1677	-86	126	1	C
ATOM	5019	C	PRO	B	29	66.733	44.847	62.108	1.00	10.21		C
ANISOU	5019	C	PRO	B	29	1336	1214	1326	-11	5	-31	C
ATOM	5020	O	PRO	B	29	67.323	44.363	63.089	1.00	9.91		O
ANISOU	5020	O	PRO	B	29	1459	1088	1217	-101	2	-85	O
ATOM	5021	N	VAL	B	30	67.017	44.568	60.839	1.00	9.27		N
ANISOU	5021	N	VAL	B	30	1201	1105	1215	19	60	77	N
ATOM	5023	CA	VAL	B	30	68.303	43.966	60.479	1.00	8.71		C
ANISOU	5023	CA	VAL	B	30	1083	1091	1134	-18	-15	23	C
ATOM	5025	CB	VAL	B	30	68.168	42.703	59.648	1.00	8.93		C
ANISOU	5025	CB	VAL	B	30	1171	959	1263	35	59	70	C
ATOM	5027	CG1	VAL	B	30	69.520	42.182	59.238	1.00	10.43		C
ANISOU	5027	CG1	VAL	B	30	1330	1166	1465	-81	65	-35	C
ATOM	5031	CG2	VAL	B	30	67.318	41.657	60.445	1.00	9.24		C
ANISOU	5031	CG2	VAL	B	30	1205	1183	1120	128	15	197	C
ATOM	5035	C	VAL	B	30	68.991	45.071	59.707	1.00	7.93		C
ANISOU	5035	C	VAL	B	30	920	1043	1050	39	4	10	C
ATOM	5090	C	LYS	B	33	64.361	46.616	58.455	1.00	8.34		C
ANISOU	5090	C	LYS	B	33	929	974	1263	-11	-12	-84	C
ATOM	5091	O	LYS	B	33	65.113	45.827	58.991	1.00	9.24		O
ANISOU	5091	O	LYS	B	33	781	1411	1315	-102	-25	-87	O
ATOM	5092	N	PRO	B	34	63.047	46.558	58.667	1.00	7.59		N
ANISOU	5092	N	PRO	B	34	970	818	1094	-84	4	-105	N
ATOM	5093	CA	PRO	B	34	62.472	45.513	59.507	1.00	8.98		C
ANISOU	5093	CA	PRO	B	34	1077	1182	1152	-23	35	-39	C

ATOM	5095	CB	PRO B	34	60.985	45.768	59.400	1.00	9.13		C
ANISOU	5095	CB	PRO B	34	1067	1116	1285	-48	23	62	C
ATOM	5098	CG	PRO B	34	60.849	47.252	59.081	1.00	10.63		C
ANISOU	5098	CG	PRO B	34	1298	1261	1479	-145	35	21	C
ATOM	5104	C	PRO B	34	62.771	44.107	59.005	1.00	7.71		C
ANISOU	5104	C	PRO B	34	816	983	1128	-25	-1	-9	C
ATOM	5105	O	PRO B	34	62.764	43.847	57.773	1.00	7.91		O
ANISOU	5105	O	PRO B	34	713	1166	1125	111	81	-8	O
ATOM	5106	N	MET B	35	63.017	43.207	59.951	1.00	7.63		N
ANISOU	5106	N	MET B	35	706	1152	1039	-122	87	-32	N
ATOM	5108	CA	MET B	35	63.328	41.808	59.621	1.00	9.13		C
ANISOU	5108	CA	MET B	35	1145	1167	1154	-49	7	-19	C
ATOM	5110	CB	MET B	35	63.300	40.920	60.858	1.00	9.98		C
ANISOU	5110	CB	MET B	35	1300	1325	1166	-82	11	-5	C
ATOM	5113	CG	MET B	35	63.864	39.465	60.653	1.00	11.02		C
ANISOU	5113	CG	MET B	35	1780	1158	1246	-345	-175	-105	C
ATOM	5116	SD	MET B	35	63.800	38.601	62.205	1.00	14.63		S
ANISOU	5116	SD	MET B	35	1523	2283	1753	-297	95	121	S
ATOM	5117	CE	MET B	35	64.826	39.520	63.177	1.00	15.95		C
ANISOU	5117	CE	MET B	35	2042	2110	1907	-184	-25	83	C
ATOM	5121	C	MET B	35	62.385	41.213	58.575	1.00	8.72		C
ANISOU	5121	C	MET B	35	1112	1140	1059	-50	19	1	C
ATOM	5122	O	MET B	35	62.867	40.538	57.670	1.00	8.66		O
ANISOU	5122	O	MET B	35	1201	1148	939	-13	2	-84	O
ATOM	5123	N	ILE B	36	61.076	41.436	58.713	1.00	8.24		N
ANISOU	5123	N	ILE B	36	1075	1059	993	-10	76	-1	N
ATOM	5125	CA	ILE B	36	60.102	40.883	57.768	1.00	8.01		C
ANISOU	5125	CA	ILE B	36	872	1072	1097	33	47	58	C
ATOM	5127	CB	ILE B	36	58.619	41.164	58.237	1.00	9.39		C
ANISOU	5127	CB	ILE B	36	1145	1265	1155	-1	83	-47	C
ATOM	5129	CG1	ILE B	36	57.741	40.087	57.611	1.00	11.66		C
ANISOU	5129	CG1	ILE B	36	1333	1657	1439	-49	-24	-111	C
ATOM	5132	CD1	ILE B	36	56.387	39.965	58.155	1.00	12.01		C
ANISOU	5132	CD1	ILE B	36	1482	1729	1350	-188	-7	-57	C
ATOM	5136	CG2	ILE B	36	58.183	42.568	57.920	1.00	11.74		C
ANISOU	5136	CG2	ILE B	36	1296	1644	1519	37	-37	-4	C
ATOM	5140	C	ILE B	36	60.336	41.218	56.285	1.00	7.69		C
ANISOU	5140	C	ILE B	36	853	973	1095	-6	66	-32	C
ATOM	5141	O	ILE B	36	59.901	40.475	55.413	1.00	8.24		O
ANISOU	5141	O	ILE B	36	1146	904	1080	-148	207	56	O
ATOM	5142	N	TYR B	37	60.947	42.386	55.989	1.00	7.41		N
ANISOU	5142	N	TYR B	37	862	1008	946	-3	113	2	N
ATOM	5144	CA	TYR B	37	61.314	42.718	54.635	1.00	6.57		C
ANISOU	5144	CA	TYR B	37	834	832	831	5	12	41	C
ATOM	5146	CB	TYR B	37	62.094	44.051	54.598	1.00	5.76		C
ANISOU	5146	CB	TYR B	37	671	937	580	20	126	-78	C
ATOM	5149	CG	TYR B	37	61.225	45.319	54.625	1.00	6.27		C
ANISOU	5149	CG	TYR B	37	763	977	640	79	-53	138	C
ATOM	5150	CD1	TYR B	37	59.977	45.362	55.285	1.00	6.67		C
ANISOU	5150	CD1	TYR B	37	689	923	922	-116	-212	178	C
ATOM	5161	C	TYR B	37	62.118	41.618	53.938	1.00	6.40		C
ANISOU	5161	C	TYR B	37	667	847	916	-119	69	37	C
ATOM	5162	O	TYR B	37	61.976	41.379	52.731	1.00	5.51		O
ANISOU	5162	O	TYR B	37	528	726	839	-18	104	-29	O
ATOM	5163	N	TYR B	38	62.957	40.932	54.685	1.00	6.74		N
ANISOU	5163	N	TYR B	38	940	848	772	-144	38	31	N
ATOM	5165	CA	TYR B	38	63.881	39.967	54.092	1.00	8.02		C
ANISOU	5165	CA	TYR B	38	992	1023	1029	-5	38	1	C
ATOM	5167	CB	TYR B	38	65.067	39.689	55.038	1.00	8.26		C
ANISOU	5167	CB	TYR B	38	1020	1040	1077	-34	123	-31	C
ATOM	5170	CG	TYR B	38	65.918	40.911	55.307	1.00	6.50		C

ANISOU	5170	CG	TYR	B	38	695	1064	710	127	-40	61	C
ATOM	5171	CD1	TYR	B	38	65.620	41.760	56.335	1.00	7.59		C
ANISOU	5171	CD1	TYR	B	38	1037	774	1070	44	-9	102	C
ATOM	5173	CE1	TYR	B	38	66.380	42.897	56.588	1.00	7.58		C
ANISOU	5173	CE1	TYR	B	38	754	1048	1077	84	-110	30	C
ATOM	5175	CZ	TYR	B	38	67.516	43.123	55.821	1.00	8.57		C
ANISOU	5175	CZ	TYR	B	38	1206	1091	960	-116	145	-54	C
ATOM	5178	CE2	TYR	B	38	67.850	42.266	54.797	1.00	10.12		C
ANISOU	5178	CE2	TYR	B	38	1517	1163	1162	41	187	-86	C
ATOM	5180	CD2	TYR	B	38	67.048	41.181	54.534	1.00	9.81		C
ANISOU	5180	CD2	TYR	B	38	1027	1419	1280	-148	71	51	C
ATOM	5182	C	TYR	B	38	63.124	38.704	53.553	1.00	9.16		C
ANISOU	5182	C	TYR	B	38	1277	1001	1200	-16	64	-2	C
ATOM	5183	O	TYR	B	38	63.177	38.411	52.348	1.00	8.72		O
ANISOU	5183	O	TYR	B	38	1364	836	1111	184	121	0	O
ATOM	5184	N	PRO	B	39	62.338	37.999	54.378	1.00	9.47		N
ANISOU	5184	N	PRO	B	39	1333	1130	1135	-73	61	1	N
ATOM	5185	CA	PRO	B	39	61.552	36.872	53.837	1.00	9.40		C
ANISOU	5185	CA	PRO	B	39	1217	1157	1197	-69	12	-31	C
ATOM	5187	CB	PRO	B	39	60.966	36.211	55.091	1.00	8.17		C
ANISOU	5187	CB	PRO	B	39	970	1021	1114	18	-26	-59	C
ATOM	5190	CG	PRO	B	39	60.977	37.302	56.148	1.00	8.67		C
ANISOU	5190	CG	PRO	B	39	1240	1077	974	-89	-81	63	C
ATOM	5193	CD	PRO	B	39	62.242	38.067	55.845	1.00	10.35		C
ANISOU	5193	CD	PRO	B	39	1374	1284	1274	-114	45	-67	C
ATOM	5196	C	PRO	B	39	60.469	37.287	52.801	1.00	9.44		C
ANISOU	5196	C	PRO	B	39	1156	1145	1285	-8	35	13	C
ATOM	5197	O	PRO	B	39	60.149	36.501	51.862	1.00	9.58		O
ANISOU	5197	O	PRO	B	39	1047	1048	1541	22	-9	12	O
ATOM	5198	N	LEU	B	40	59.917	38.495	52.964	1.00	8.59		N
ANISOU	5198	N	LEU	B	40	1006	1121	1136	-54	144	60	N
ATOM	5200	CA	LEU	B	40	58.945	39.015	52.060	1.00	8.88		C
ANISOU	5200	CA	LEU	B	40	1124	1117	1132	-19	92	67	C
ATOM	5202	CB	LEU	B	40	58.462	40.389	52.565	1.00	8.20		C
ANISOU	5202	CB	LEU	B	40	1099	1127	888	-26	95	36	C
ATOM	5205	CG	LEU	B	40	57.606	41.124	51.517	1.00	10.43		C
ANISOU	5205	CG	LEU	B	40	1296	1268	1398	23	36	10	C
ATOM	5207	CD1	LEU	B	40	56.432	40.286	51.194	1.00	12.24		C
ANISOU	5207	CD1	LEU	B	40	1421	1546	1683	72	109	-192	C
ATOM	5211	CD2	LEU	B	40	57.186	42.500	51.998	1.00	10.51		C
ANISOU	5211	CD2	LEU	B	40	1163	1479	1348	32	-25	-2	C
ATOM	5215	C	LEU	B	40	59.616	39.162	50.677	1.00	9.80		C
ANISOU	5215	C	LEU	B	40	1282	1260	1180	84	11	26	C
ATOM	5216	O	LEU	B	40	59.108	38.692	49.649	1.00	8.59		O
ANISOU	5216	O	LEU	B	40	1091	1004	1167	245	-53	-19	O
ATOM	5217	N	SER	B	41	60.791	39.769	50.695	1.00	10.05		N
ANISOU	5217	N	SER	B	41	1352	1208	1258	-22	6	37	N
ATOM	5219	CA	SER	B	41	61.610	39.892	49.501	1.00	10.26		C
ANISOU	5219	CA	SER	B	41	1399	1306	1194	78	5	0	C
ATOM	5224	OG	SER	B	41	64.043	39.812	50.309	1.00	12.34		O
ANISOU	5224	OG	SER	B	41	1173	1758	1757	-134	-105	-71	O
ATOM	5226	C	SER	B	41	61.897	38.523	48.816	1.00	10.05		C
ANISOU	5226	C	SER	B	41	1325	1231	1263	26	-2	0	C
ATOM	5228	N	THR	B	42	62.099	37.494	49.625	1.00	8.33		N
ANISOU	5228	N	THR	B	42	985	1187	991	1	63	17	N
ATOM	5230	CA	THR	B	42	62.379	36.162	49.122	1.00	8.14		C
ANISOU	5230	CA	THR	B	42	907	1146	1040	-54	52	-17	C
ATOM	5232	CB	THR	B	42	62.784	35.260	50.254	1.00	8.33		C
ANISOU	5232	CB	THR	B	42	869	1263	1033	5	19	-75	C
ATOM	5234	OG1	THR	B	42	64.133	35.579	50.714	1.00	9.46		O
ANISOU	5234	OG1	THR	B	42	873	1479	1239	32	-198	-150	O

ATOM	5236	CG2	THR	B	42	62.799	33.833	49.839	1.00	9.75		C
ANISOU	5236	CG2	THR	B	42	1166	1363	1174	-27	23	105	C
ATOM	5240	C	THR	B	42	61.167	35.625	48.327	1.00	8.32		C
ANISOU	5240	C	THR	B	42	991	1127	1041	-50	44	12	C
ATOM	5242	N	LEU	B	43	59.992	35.709	48.907	1.00	8.39		N
ANISOU	5242	N	LEU	B	43	984	1047	1156	47	82	37	N
ATOM	5244	CA	LEU	B	43	58.798	35.361	48.143	1.00	7.89		C
ANISOU	5244	CA	LEU	B	43	1050	962	987	-17	47	-52	C
ATOM	5246	CB	LEU	B	43	57.575	35.459	49.014	1.00	7.75		C
ANISOU	5246	CB	LEU	B	43	886	945	1113	77	64	-85	C
ATOM	5249	CG	LEU	B	43	57.550	34.563	50.258	1.00	8.26		C
ANISOU	5249	CG	LEU	B	43	874	1120	1143	-6	1	-27	C
ATOM	5251	CD1	LEU	B	43	56.172	34.819	50.988	1.00	10.56		C
ANISOU	5251	CD1	LEU	B	43	1282	1449	1281	-46	130	-24	C
ATOM	5255	CD2	LEU	B	43	57.674	33.086	49.916	1.00	10.22		C
ANISOU	5255	CD2	LEU	B	43	1340	1421	1120	88	74	-2	C
ATOM	5374	CA	ILE	B	51	51.084	36.450	50.452	1.00	7.96		C
ANISOU	5374	CA	ILE	B	51	949	989	1085	9	41	31	C
ATOM	5376	CB	ILE	B	51	52.425	37.184	50.586	1.00	8.70		C
ANISOU	5376	CB	ILE	B	51	1184	996	1124	38	33	-22	C
ATOM	5385	CG2	ILE	B	51	53.101	36.831	51.886	1.00	9.88		C
ANISOU	5385	CG2	ILE	B	51	1051	1327	1375	-98	108	59	C
ATOM	5389	C	ILE	B	51	50.267	36.649	51.721	1.00	8.56		C
ANISOU	5389	C	ILE	B	51	1107	1075	1070	105	-24	-22	C
ATOM	5390	O	ILE	B	51	49.738	37.768	52.001	1.00	8.21		O
ANISOU	5390	O	ILE	B	51	1080	1144	894	210	-106	-81	O
ATOM	5391	N	LEU	B	52	50.161	35.569	52.484	1.00	8.46		N
ANISOU	5391	N	LEU	B	52	912	1127	1172	85	10	-8	N
ATOM	5393	CA	LEU	B	52	49.565	35.575	53.807	1.00	8.24		C
ANISOU	5393	CA	LEU	B	52	1001	1062	1067	40	24	6	C
ATOM	5395	CB	LEU	B	52	48.754	34.291	53.982	1.00	8.67		C
ANISOU	5395	CB	LEU	B	52	1178	1014	1101	77	57	18	C
ATOM	5398	CG	LEU	B	52	48.054	34.060	55.339	1.00	7.53		C
ANISOU	5398	CG	LEU	B	52	927	1041	892	33	-43	8	C
ATOM	5400	CD1	LEU	B	52	46.944	35.069	55.573	1.00	8.59		C
ANISOU	5400	CD1	LEU	B	52	1101	1105	1056	-86	337	62	C
ATOM	5404	CD2	LEU	B	52	47.521	32.680	55.511	1.00	8.31		C
ANISOU	5404	CD2	LEU	B	52	960	1189	1008	166	49	-134	C
ATOM	5408	C	LEU	B	52	50.635	35.654	54.883	1.00	8.13		C
ANISOU	5408	C	LEU	B	52	999	958	1129	19	70	10	C
ATOM	5409	O	LEU	B	52	51.626	34.852	54.886	1.00	9.12		O
ANISOU	5409	O	LEU	B	52	1034	1130	1300	294	32	-3	O
ATOM	5410	N	ILE	B	53	50.484	36.634	55.776	1.00	7.32		N
ANISOU	5410	N	ILE	B	53	919	990	871	71	131	43	N
ATOM	5412	CA	ILE	B	53	51.421	36.851	56.886	1.00	7.74		C
ANISOU	5412	CA	ILE	B	53	977	964	997	38	86	27	C
ATOM	5414	CB	ILE	B	53	51.817	38.309	56.986	1.00	8.49		C
ANISOU	5414	CB	ILE	B	53	1166	1046	1013	-6	30	-30	C
ATOM	5416	CG1	ILE	B	53	52.598	38.707	55.730	1.00	10.63		C
ANISOU	5416	CG1	ILE	B	53	1234	1289	1512	-14	90	100	C
ATOM	5419	CD1	ILE	B	53	52.807	40.069	55.625	1.00	13.20		C
ANISOU	5419	CD1	ILE	B	53	1748	1539	1726	-85	202	1	C
ATOM	5423	CG2	ILE	B	53	52.616	38.568	58.211	1.00	8.69		C
ANISOU	5423	CG2	ILE	B	53	1074	1006	1221	12	-70	24	C
ATOM	5427	C	ILE	B	53	50.725	36.389	58.134	1.00	7.77		C
ANISOU	5427	C	ILE	B	53	1021	1001	929	35	49	-30	C
ATOM	5428	O	ILE	B	53	49.630	36.892	58.492	1.00	7.32		O
ANISOU	5428	O	ILE	B	53	928	969	883	-11	2	81	O
ATOM	5429	N	ILE	B	54	51.310	35.350	58.720	1.00	8.14		N
ANISOU	5429	N	ILE	B	54	911	1174	1005	38	39	45	N
ATOM	5431	CA	ILE	B	54	50.812	34.787	59.936	1.00	9.27		C

ANISOU	5431	CA	ILE	B	54	1091	1292	1136	2	61	15	C
ATOM	5433	CB	ILE	B	54	50.743	33.260	59.869	1.00	8.45		C
ANISOU	5433	CB	ILE	B	54	997	1241	970	-9	137	-23	C
ATOM	5435	CG1	ILE	B	54	49.809	32.847	58.725	1.00	9.41		C
ANISOU	5435	CG1	ILE	B	54	1015	1221	1339	34	5	99	C
ATOM	5438	CD1	ILE	B	54	49.762	31.413	58.454	1.00	9.26		C
ANISOU	5438	CD1	ILE	B	54	1132	1327	1056	-31	23	32	C
ATOM	5442	CG2	ILE	B	54	50.268	32.690	61.194	1.00	8.94		C
ANISOU	5442	CG2	ILE	B	54	1254	1152	991	-81	74	-158	C
ATOM	5446	C	ILE	B	54	51.628	35.258	61.121	1.00	9.49		C
ANISOU	5446	C	ILE	B	54	1065	1318	1222	-31	14	0	C
ATOM	5447	O	ILE	B	54	52.850	35.189	61.105	1.00	10.96		O
ANISOU	5447	O	ILE	B	54	1177	1581	1406	146	108	-47	O
ATOM	5448	N	SER	B	55	50.942	35.752	62.147	1.00	8.46		N
ANISOU	5448	N	SER	B	55	948	1105	1162	3	-25	-34	N
ATOM	5450	CA	SER	B	55	51.604	36.172	63.361	1.00	8.73		C
ANISOU	5450	CA	SER	B	55	1070	1142	1104	70	-16	40	C
ATOM	5452	CB	SER	B	55	52.151	37.586	63.282	1.00	8.67		C
ANISOU	5452	CB	SER	B	55	1042	1193	1058	-1	42	37	C
ATOM	5455	OG	SER	B	55	53.131	37.809	64.325	1.00	13.77		O
ANISOU	5455	OG	SER	B	55	1638	1951	1640	260	-4	-247	O
ATOM	5457	C	SER	B	55	50.729	35.916	64.604	1.00	8.11		C
ANISOU	5457	C	SER	B	55	834	1177	1068	71	59	-85	C
ATOM	5458	O	SER	B	55	49.690	35.226	64.541	1.00	7.60		O
ANISOU	5458	O	SER	B	55	765	1202	921	198	-149	-9	O
ATOM	5459	N	THR	B	56	51.268	36.289	65.740	1.00	8.14		N
ANISOU	5459	N	THR	B	56	747	1172	1170	-27	3	-68	N
ATOM	5461	CA	THR	B	56	50.593	36.155	66.977	1.00	8.46		C
ANISOU	5461	CA	THR	B	56	993	1166	1052	-59	-3	-4	C
ATOM	5463	CB	THR	B	56	51.456	36.546	68.219	1.00	8.45		C
ANISOU	5463	CB	THR	B	56	837	1109	1261	-48	-17	-13	C
ATOM	5465	OG1	THR	B	56	51.823	37.916	68.140	1.00	8.18		O
ANISOU	5465	OG1	THR	B	56	673	1239	1193	-211	14	-72	O
ATOM	5467	CG2	THR	B	56	52.690	35.717	68.381	1.00	8.38		C
ANISOU	5467	CG2	THR	B	56	896	1123	1165	-50	-166	54	C
ATOM	5471	C	THR	B	56	49.396	37.092	67.002	1.00	8.49		C
ANISOU	5471	C	THR	B	56	835	1182	1207	13	-73	20	C
ATOM	5472	O	THR	B	56	49.310	38.055	66.229	1.00	9.15		O
ANISOU	5472	O	THR	B	56	870	1418	1188	-94	72	-13	O
ATOM	5473	N	PRO	B	57	48.475	36.899	67.924	1.00	9.92		N
ANISOU	5473	N	PRO	B	57	1184	1287	1296	1	5	40	N
ATOM	5474	CA	PRO	B	57	47.374	37.862	67.966	1.00	10.34		C
ANISOU	5474	CA	PRO	B	57	1147	1341	1437	-22	2	47	C
ATOM	5476	CB	PRO	B	57	46.468	37.335	69.114	1.00	10.65		C
ANISOU	5476	CB	PRO	B	57	1334	1382	1329	47	70	9	C
ATOM	5479	CG	PRO	B	57	46.849	35.898	69.207	1.00	12.15		C
ANISOU	5479	CG	PRO	B	57	1646	1516	1454	-80	112	88	C
ATOM	5482	CD	PRO	B	57	48.269	35.810	68.893	1.00	10.25		C
ANISOU	5482	CD	PRO	B	57	1179	1238	1476	87	-110	0	C
ATOM	5485	C	PRO	B	57	47.793	39.276	68.226	1.00	10.09		C
ANISOU	5485	C	PRO	B	57	1130	1350	1350	26	92	2	C
ATOM	5486	O	PRO	B	57	47.269	40.136	67.586	1.00	9.04		O
ANISOU	5486	O	PRO	B	57	950	1294	1189	-240	-42	135	O
ATOM	5487	N	GLN	B	58	48.770	39.505	69.092	1.00	11.87		N
ANISOU	5487	N	GLN	B	58	1525	1550	1434	55	-19	-26	N
ATOM	5489	CA	GLN	B	58	49.196	40.862	69.443	1.00	14.41		C
ANISOU	5489	CA	GLN	B	58	1816	1859	1799	13	-11	-6	C
ATOM	5491	CB	GLN	B	58	49.987	40.857	70.796	1.00	15.87		C
ANISOU	5491	CB	GLN	B	58	1992	2028	2007	42	-94	0	C
ATOM	5494	CG	GLN	B	58	51.339	40.228	70.688	1.00	19.01		C
ANISOU	5494	CG	GLN	B	58	2329	2467	2424	116	-5	42	C

ATOM	5497	CD	GLN	B	58	51.329	38.693	71.012	1.00	23.61		C
ANISOU	5497	CD	GLN	B	58	3019	2751	3200	-19	-33	94	C
ATOM	5498	OE1	GLN	B	58	50.245	38.016	70.990	1.00	22.34		O
ANISOU	5498	OE1	GLN	B	58	2795	3342	2348	-67	121	-19	O
ATOM	5499	NE2	GLN	B	58	52.549	38.137	71.275	1.00	23.63		N
ANISOU	5499	NE2	GLN	B	58	2829	3109	3038	41	-165	-25	N
ATOM	5502	C	GLN	B	58	50.036	41.528	68.370	1.00	13.95		C
ANISOU	5502	C	GLN	B	58	1667	1803	1827	13	6	19	C
ATOM	5503	O	GLN	B	58	50.089	42.735	68.288	1.00	14.86		O
ANISOU	5503	O	GLN	B	58	1794	1858	1992	76	103	16	O
ATOM	5504	N	ASP	B	59	50.712	40.742	67.553	1.00	14.39		N
ANISOU	5504	N	ASP	B	59	1845	1836	1785	-15	-5	-14	N
ATOM	5506	CA	ASP	B	59	51.645	41.332	66.575	1.00	13.88		C
ANISOU	5506	CA	ASP	B	59	1774	1710	1789	7	33	-22	C
ATOM	5508	CB	ASP	B	59	52.874	40.486	66.413	1.00	13.83		C
ANISOU	5508	CB	ASP	B	59	1677	1809	1768	-22	29	-25	C
ATOM	5511	CG	ASP	B	59	53.709	40.483	67.649	1.00	17.18		C
ANISOU	5511	CG	ASP	B	59	2013	2276	2238	-75	-176	35	C
ATOM	5512	OD1	ASP	B	59	54.145	41.604	68.007	1.00	19.30		O
ANISOU	5512	OD1	ASP	B	59	2295	2293	2746	239	-275	-218	O
ATOM	5513	OD2	ASP	B	59	53.944	39.422	68.309	1.00	16.82		O
ANISOU	5513	OD2	ASP	B	59	1632	2429	2330	-89	-408	59	O
ATOM	5514	C	ASP	B	59	51.008	41.507	65.255	1.00	13.43		C
ANISOU	5514	C	ASP	B	59	1681	1742	1680	42	52	-44	C
ATOM	5515	O	ASP	B	59	51.442	42.288	64.465	1.00	13.54		O
ANISOU	5515	O	ASP	B	59	1813	1634	1695	46	-31	64	O
ATOM	5516	N	THR	B	60	49.962	40.762	65.009	1.00	14.48		N
ANISOU	5516	N	THR	B	60	1928	1872	1701	-27	69	-69	N
ATOM	5518	CA	THR	B	60	49.296	40.874	63.715	1.00	15.28		C
ANISOU	5518	CA	THR	B	60	1925	2036	1841	-13	-17	-4	C
ATOM	5520	CB	THR	B	60	48.065	39.976	63.649	1.00	15.25		C
ANISOU	5520	CB	THR	B	60	1890	2040	1863	-1	33	-67	C
ATOM	5522	OG1	THR	B	60	48.416	38.583	63.562	1.00	15.64		O
ANISOU	5522	OG1	THR	B	60	1672	2323	1948	-52	-2	8	O
ATOM	5524	CG2	THR	B	60	47.327	40.272	62.352	1.00	15.83		C
ANISOU	5524	CG2	THR	B	60	1941	2113	1962	-58	-82	52	C
ATOM	5528	C	THR	B	60	48.946	42.335	63.323	1.00	15.48		C
ANISOU	5528	C	THR	B	60	2032	1957	1890	-43	2	-80	C
ATOM	5529	O	THR	B	60	49.275	42.805	62.216	1.00	15.73		O
ANISOU	5529	O	THR	B	60	2196	2032	1748	-86	67	-79	O
ATOM	5530	N	PRO	B	61	48.339	43.108	64.204	1.00	15.22		N
ANISOU	5530	N	PRO	B	61	1873	2044	1865	-14	113	2	N
ATOM	5531	CA	PRO	B	61	48.018	44.498	63.847	1.00	15.29		C
ANISOU	5531	CA	PRO	B	61	1906	1998	1904	28	73	-21	C
ATOM	5536	CG	PRO	B	61	46.840	43.719	65.774	1.00	15.26		C
ANISOU	5536	CG	PRO	B	61	1788	2061	1946	37	119	28	C
ATOM	5539	CD	PRO	B	61	47.910	42.752	65.559	1.00	16.01		C
ANISOU	5539	CD	PRO	B	61	2094	2027	1959	-3	-2	-1	C
ATOM	5542	C	PRO	B	61	49.270	45.361	63.602	1.00	15.54		C
ANISOU	5542	C	PRO	B	61	1936	2023	1945	84	85	-39	C
ATOM	5544	N	ARG	B	62	50.386	44.953	64.170	1.00	15.87		N
ANISOU	5544	N	ARG	B	62	1985	2129	1914	55	6	-9	N
ATOM	5546	CA	ARG	B	62	51.613	45.727	63.973	1.00	15.78		C
ANISOU	5546	CA	ARG	B	62	1973	2019	2001	34	63	-23	C
ATOM	5548	CB	ARG	B	62	52.648	45.354	65.012	1.00	16.56		C
ANISOU	5548	CB	ARG	B	62	2052	2145	2093	-33	16	-42	C
ATOM	5551	CG	ARG	B	62	52.135	45.380	66.432	1.00	21.36		C
ANISOU	5551	CG	ARG	B	62	2819	2687	2609	0	44	-15	C
ATOM	5554	CD	ARG	B	62	53.207	45.355	67.475	1.00	24.85		C
ANISOU	5554	CD	ARG	B	62	3140	3144	3157	-68	-140	59	C
ATOM	5557	NE	ARG	B	62	52.576	45.498	68.786	1.00	29.42		N

ANISOU	5557	NE	ARG	B	62	3763	3767	3648	90	81	-43	N
ATOM	5559	CZ	ARG	B	62	52.591	44.583	69.758	1.00	31.69		C
ANISOU	5559	CZ	ARG	B	62	4093	3979	3967	-32	-2	55	C
ATOM	5560	NH1	ARG	B	62	53.245	43.426	69.621	1.00	31.75		N
ANISOU	5560	NH1	ARG	B	62	3953	4091	4019	57	-2	85	N
ATOM	5566	C	ARG	B	62	52.138	45.467	62.552	1.00	15.23		C
ANISOU	5566	C	ARG	B	62	1861	1997	1928	9	-39	16	C
ATOM	5567	O	ARG	B	62	52.666	46.357	61.875	1.00	14.60		O
ANISOU	5567	O	ARG	B	62	1885	1838	1824	138	3	49	O
ATOM	5568	N	PHE	B	63	52.032	44.239	62.103	1.00	14.42		N
ANISOU	5568	N	PHE	B	63	1762	1881	1835	24	1	-30	N
ATOM	5570	CA	PHE	B	63	52.434	43.988	60.730	1.00	14.37		C
ANISOU	5570	CA	PHE	B	63	1812	1847	1800	-26	39	61	C
ATOM	5572	CB	PHE	B	63	52.532	42.512	60.442	1.00	14.23		C
ANISOU	5572	CB	PHE	B	63	1706	1816	1884	-38	61	44	C
ATOM	5575	CG	PHE	B	63	53.669	41.851	61.120	1.00	14.00		C
ANISOU	5575	CG	PHE	B	63	1775	1805	1737	-67	10	35	C
ATOM	5576	CD1	PHE	B	63	53.469	41.123	62.270	1.00	14.72		C
ANISOU	5576	CD1	PHE	B	63	1913	1808	1871	238	179	81	C
ATOM	5578	CE1	PHE	B	63	54.507	40.516	62.917	1.00	15.76		C
ANISOU	5578	CE1	PHE	B	63	1851	2147	1989	-150	-35	188	C
ATOM	5580	CZ	PHE	B	63	55.765	40.618	62.449	1.00	15.25		C
ANISOU	5580	CZ	PHE	B	63	1838	2072	1884	221	176	118	C
ATOM	5582	CE2	PHE	B	63	55.992	41.391	61.319	1.00	18.17		C
ANISOU	5582	CE2	PHE	B	63	2331	2417	2152	171	127	222	C
ATOM	5584	CD2	PHE	B	63	54.932	41.983	60.644	1.00	14.15		C
ANISOU	5584	CD2	PHE	B	63	1678	2026	1671	93	118	94	C
ATOM	5586	C	PHE	B	63	51.458	44.678	59.758	1.00	13.76		C
ANISOU	5586	C	PHE	B	63	1674	1784	1768	1	32	47	C
ATOM	5587	O	PHE	B	63	51.861	45.219	58.719	1.00	12.02		O
ANISOU	5587	O	PHE	B	63	1667	1384	1514	-27	74	96	O
ATOM	5588	N	GLN	B	64	50.170	44.624	60.060	1.00	13.88		N
ANISOU	5588	N	GLN	B	64	1702	1766	1804	27	73	19	N
ATOM	5635	CD2	LEU	B	66	57.020	46.274	58.876	1.00	14.82		C
ANISOU	5635	CD2	LEU	B	66	1778	1960	1890	0	-109	122	C
ATOM	5648	CG	LEU	B	67	54.382	44.799	55.922	1.00	13.29		C
ANISOU	5648	CG	LEU	B	67	1725	1771	1552	-68	22	33	C
ATOM	5650	CD1	LEU	B	67	54.540	43.319	56.140	1.00	13.39		C
ANISOU	5650	CD1	LEU	B	67	1732	1603	1751	-23	-51	-6	C
ATOM	5807	C	GLN	B	78	47.225	38.787	55.119	1.00	8.92		C
ANISOU	5807	C	GLN	B	78	1067	1219	1102	-10	8	-62	C
ATOM	5808	O	GLN	B	78	48.410	38.488	55.143	1.00	8.25		O
ANISOU	5808	O	GLN	B	78	1025	1038	1070	88	241	-162	O
ATOM	5809	N	TYR	B	79	46.428	38.709	56.177	1.00	8.99		N
ANISOU	5809	N	TYR	B	79	1002	1248	1165	74	55	-3	N
ATOM	5811	CA	TYR	B	79	46.895	38.435	57.488	1.00	8.02		C
ANISOU	5811	CA	TYR	B	79	839	1137	1070	54	1	-1	C
ATOM	5813	CB	TYR	B	79	46.950	39.767	58.265	1.00	8.97		C
ANISOU	5813	CB	TYR	B	79	1017	1308	1081	28	-40	50	C
ATOM	5816	CG	TYR	B	79	47.829	40.783	57.637	1.00	10.67		C
ANISOU	5816	CG	TYR	B	79	1470	1218	1366	33	-75	-29	C
ATOM	5817	CD1	TYR	B	79	47.372	41.585	56.591	1.00	10.41		C
ANISOU	5817	CD1	TYR	B	79	1287	1434	1233	48	-23	53	C
ATOM	5821	CZ	TYR	B	79	49.508	42.647	56.456	1.00	11.42		C
ANISOU	5821	CZ	TYR	B	79	1639	1375	1323	23	-103	73	C
ATOM	5824	CE2	TYR	B	79	49.983	41.862	57.492	1.00	13.23		C
ANISOU	5824	CE2	TYR	B	79	1691	1689	1643	97	-35	125	C
ATOM	5826	CD2	TYR	B	79	49.149	40.954	58.078	1.00	10.33		C
ANISOU	5826	CD2	TYR	B	79	1290	1228	1406	121	-37	68	C
ATOM	5828	C	TYR	B	79	45.968	37.423	58.190	1.00	9.02		C
ANISOU	5828	C	TYR	B	79	968	1329	1128	34	-5	41	C

ATOM	5829	O	TYR	B	79	44.711	37.440	57.977	1.00	9.52		O
ANISOU	5829	O	TYR	B	79	773	1538	1304	14	55	65	O
ATOM	5830	N	ALA	B	80	46.571	36.536	58.984	1.00	7.80		N
ANISOU	5830	N	ALA	B	80	819	1031	1112	115	44	12	N
ATOM	5832	CA	ALA	B	80	45.854	35.619	59.849	1.00	8.40		C
ANISOU	5832	CA	ALA	B	80	998	1151	1041	66	-4	9	C
ATOM	5834	CB	ALA	B	80	45.566	34.241	59.164	1.00	7.99		C
ANISOU	5834	CB	ALA	B	80	828	1188	1018	-9	-9	35	C
ATOM	5838	C	ALA	B	80	46.657	35.400	61.149	1.00	9.34		C
ANISOU	5838	C	ALA	B	80	1149	1279	1120	16	-36	49	C
ATOM	5839	O	ALA	B	80	47.867	35.540	61.200	1.00	8.68		O
ANISOU	5839	O	ALA	B	80	1091	1323	884	239	-125	131	O
ATOM	5840	N	VAL	B	81	45.926	35.078	62.194	1.00	9.78		N
ANISOU	5840	N	VAL	B	81	1170	1395	1151	56	3	33	N
ATOM	5842	CA	VAL	B	81	46.490	34.876	63.510	1.00	10.70		C
ANISOU	5842	CA	VAL	B	81	1382	1466	1217	-1	-3	-18	C
ATOM	5844	CB	VAL	B	81	45.440	35.381	64.540	1.00	10.77		C
ANISOU	5844	CB	VAL	B	81	1355	1459	1275	73	-125	-40	C
ATOM	5846	CG1	VAL	B	81	45.844	34.991	65.963	1.00	15.07		C
ANISOU	5846	CG1	VAL	B	81	2122	2004	1596	-12	8	10	C
ATOM	5850	CG2	VAL	B	81	45.255	36.854	64.391	1.00	11.08		C
ANISOU	5850	CG2	VAL	B	81	1359	1557	1291	-7	-5	-129	C
ATOM	5854	C	VAL	B	81	46.766	33.405	63.798	1.00	10.54		C
ANISOU	5854	C	VAL	B	81	1348	1426	1231	-36	17	-5	C
ATOM	5855	O	VAL	B	81	45.964	32.542	63.439	1.00	10.69		O
ANISOU	5855	O	VAL	B	81	1345	1493	1224	-170	-151	-83	O
ATOM	5856	N	GLN	B	82	47.911	33.116	64.414	1.00	10.66		N
ANISOU	5856	N	GLN	B	82	1423	1342	1284	-102	25	22	N
ATOM	5858	CA	GLN	B	82	48.188	31.819	65.022	1.00	10.04		C
ANISOU	5858	CA	GLN	B	82	1313	1268	1234	13	-5	38	C
ATOM	5860	CB	GLN	B	82	49.594	31.337	64.689	1.00	9.48		C
ANISOU	5860	CB	GLN	B	82	1232	1262	1107	-46	127	70	C
ATOM	5863	CG	GLN	B	82	49.974	30.000	65.256	1.00	7.09		C
ANISOU	5863	CG	GLN	B	82	1047	1081	563	-69	230	-8	C
ATOM	5866	CD	GLN	B	82	51.323	29.560	64.910	1.00	8.66		C
ANISOU	5866	CD	GLN	B	82	1307	1041	939	-4	29	123	C
ATOM	5867	OE1	GLN	B	82	52.258	30.389	64.823	1.00	10.82		O
ANISOU	5867	OE1	GLN	B	82	1045	1502	1562	156	105	-69	O
ATOM	5868	NE2	GLN	B	82	51.485	28.221	64.712	1.00	11.05		N
ANISOU	5868	NE2	GLN	B	82	1410	1351	1437	57	110	-109	N
ATOM	5871	C	GLN	B	82	48.008	32.004	66.552	1.00	10.14		C
ANISOU	5871	C	GLN	B	82	1375	1204	1270	19	-74	21	C
ATOM	5872	O	GLN	B	82	48.691	32.824	67.151	1.00	8.93		O
ANISOU	5872	O	GLN	B	82	930	1355	1106	13	-342	210	O
ATOM	5873	N	PRO	B	83	47.032	31.342	67.180	1.00	11.13		N
ANISOU	5873	N	PRO	B	83	1383	1422	1424	65	-79	9	N
ATOM	5874	CA	PRO	B	83	46.794	31.558	68.615	1.00	12.40		C
ANISOU	5874	CA	PRO	B	83	1564	1595	1549	5	-2	53	C
ATOM	5876	CB	PRO	B	83	45.618	30.622	68.920	1.00	12.26		C
ANISOU	5876	CB	PRO	B	83	1470	1634	1555	0	-4	12	C
ATOM	5879	CG	PRO	B	83	44.973	30.361	67.633	1.00	12.89		C
ANISOU	5879	CG	PRO	B	83	1616	1658	1623	84	-42	14	C
ATOM	5882	CD	PRO	B	83	45.992	30.469	66.589	1.00	11.71		C
ANISOU	5882	CD	PRO	B	83	1617	1235	1594	-4	18	67	C
ATOM	5885	C	PRO	B	83	47.988	31.235	69.504	1.00	12.77		C
ANISOU	5885	C	PRO	B	83	1594	1684	1572	-2	8	26	C
ATOM	5886	O	PRO	B	83	48.290	31.988	70.456	1.00	13.42		O
ANISOU	5886	O	PRO	B	83	1641	1795	1663	10	117	-64	O
ATOM	5887	N	SER	B	84	48.688	30.162	69.172	1.00	12.21		N
ANISOU	5887	N	SER	B	84	1531	1614	1495	3	26	28	N
ATOM	5889	CA	SER	B	84	49.863	29.755	69.930	1.00	12.54		C

ANISOU	5889	CA	SER	B	84	1536	1619	1608	81	-27	15	C
ATOM	5891	CB	SER	B	84	49.444	28.734	70.964	1.00	12.66		C
ANISOU	5891	CB	SER	B	84	1490	1737	1582	44	12	14	C
ATOM	5894	OG	SER	B	84	50.498	28.512	71.895	1.00	18.45		O
ANISOU	5894	OG	SER	B	84	2286	2435	2286	184	-178	177	O
ATOM	5896	C	SER	B	84	50.889	29.158	68.970	1.00	11.40		C
ANISOU	5896	C	SER	B	84	1325	1552	1452	-4	30	33	C
ATOM	5897	O	SER	B	84	50.519	28.540	68.005	1.00	9.30		O
ANISOU	5897	O	SER	B	84	640	1614	1277	283	-63	121	O
ATOM	5898	N	PRO	B	85	52.177	29.291	69.256	1.00	12.42		N
ANISOU	5898	N	PRO	B	85	1526	1648	1544	97	-156	-57	N
ATOM	5899	CA	PRO	B	85	53.217	28.842	68.342	1.00	12.47		C
ANISOU	5899	CA	PRO	B	85	1467	1686	1582	43	-119	22	C
ATOM	5901	CB	PRO	B	85	54.462	29.635	68.802	1.00	13.15		C
ANISOU	5901	CB	PRO	B	85	1596	1680	1720	110	-152	-22	C
ATOM	5904	CG	PRO	B	85	54.231	29.887	70.211	1.00	14.30		C
ANISOU	5904	CG	PRO	B	85	1671	1984	1777	0	-14	17	C
ATOM	5907	CD	PRO	B	85	52.730	29.931	70.461	1.00	13.75		C
ANISOU	5907	CD	PRO	B	85	1689	1882	1653	90	-149	-11	C
ATOM	5910	C	PRO	B	85	53.397	27.317	68.465	1.00	12.17		C
ANISOU	5910	C	PRO	B	85	1455	1641	1525	78	-53	-40	C
ATOM	5911	O	PRO	B	85	54.399	26.805	68.968	1.00	12.15		O
ANISOU	5911	O	PRO	B	85	1560	1608	1447	248	-205	-8	O
ATOM	5912	N	ASP	B	86	52.403	26.612	67.976	1.00	10.80		N
ANISOU	5912	N	ASP	B	86	1346	1566	1190	71	73	-58	N
ATOM	5914	CA	ASP	B	86	52.321	25.228	68.124	1.00	11.92		C
ANISOU	5914	CA	ASP	B	86	1467	1571	1489	91	28	-10	C
ATOM	5916	CB	ASP	B	86	50.908	24.816	68.556	1.00	13.23		C
ANISOU	5916	CB	ASP	B	86	1610	1710	1707	14	21	-1	C
ATOM	5919	CG	ASP	B	86	50.524	25.368	69.911	1.00	16.05		C
ANISOU	5919	CG	ASP	B	86	1988	2059	2050	117	11	-27	C
ATOM	5920	OD1	ASP	B	86	51.380	25.878	70.662	1.00	18.77		O
ANISOU	5920	OD1	ASP	B	86	2721	2285	2124	10	-163	-105	O
ATOM	5921	OD2	ASP	B	86	49.347	25.373	70.284	1.00	20.09		O
ANISOU	5921	OD2	ASP	B	86	2402	2714	2517	-259	571	94	O
ATOM	5922	C	ASP	B	86	52.749	24.456	66.903	1.00	10.99		C
ANISOU	5922	C	ASP	B	86	1304	1560	1311	-24	-41	4	C
ATOM	5923	O	ASP	B	86	52.488	23.239	66.792	1.00	10.78		O
ANISOU	5923	O	ASP	B	86	1135	1522	1437	107	27	18	O
ATOM	5924	N	GLY	B	87	53.509	25.127	66.039	1.00	10.42		N
ANISOU	5924	N	GLY	B	87	1385	1337	1237	-49	-58	-38	N
ATOM	5926	CA	GLY	B	87	54.169	24.415	64.992	1.00	10.02		C
ANISOU	5926	CA	GLY	B	87	1194	1298	1314	19	34	-33	C
ATOM	5929	C	GLY	B	87	54.118	25.023	63.635	1.00	9.38		C
ANISOU	5929	C	GLY	B	87	1162	1219	1180	20	-32	-52	C
ATOM	5930	O	GLY	B	87	53.076	25.566	63.254	1.00	9.96		O
ANISOU	5930	O	GLY	B	87	1142	1342	1298	58	-10	-221	O
ATOM	5931	N	LEU	B	88	55.211	24.879	62.865	1.00	8.48		N
ANISOU	5931	N	LEU	B	88	822	1253	1145	80	-33	-16	N
ATOM	5933	CA	LEU	B	88	55.203	25.427	61.519	1.00	8.82		C
ANISOU	5933	CA	LEU	B	88	1060	1136	1154	7	23	14	C
ATOM	5935	CB	LEU	B	88	56.572	25.229	60.799	1.00	10.10		C
ANISOU	5935	CB	LEU	B	88	1193	1479	1165	247	-69	117	C
ATOM	5938	CG	LEU	B	88	57.905	25.603	61.452	1.00	14.21		C
ANISOU	5938	CG	LEU	B	88	1630	1663	2104	-107	144	-172	C
ATOM	5940	CD1	LEU	B	88	58.993	25.661	60.326	1.00	14.60		C
ANISOU	5940	CD1	LEU	B	88	2193	1639	1711	-54	212	-33	C
ATOM	5944	CD2	LEU	B	88	58.016	26.696	62.462	1.00	14.11		C
ANISOU	5944	CD2	LEU	B	88	1655	2028	1677	-186	141	-42	C
ATOM	5948	C	LEU	B	88	54.082	24.864	60.625	1.00	9.53		C
ANISOU	5948	C	LEU	B	88	1173	1222	1222	69	-14	23	C

ATOM	5949	O	LEU	B	88	53.530	25.574	59.786	1.00	10.11		O
ANISOU	5949	O	LEU	B	88	1371	1282	1185	-31	-118	18	O
ATOM	5950	N	ALA	B	89	53.706	23.606	60.819	1.00	8.94		N
ANISOU	5950	N	ALA	B	89	1045	1132	1218	91	-150	0	N
ATOM	5952	CA	ALA	B	89	52.765	22.981	59.902	1.00	9.57		C
ANISOU	5952	CA	ALA	B	89	1212	1224	1199	55	-3	-3	C
ATOM	5954	CB	ALA	B	89	52.767	21.503	60.034	1.00	9.73		C
ANISOU	5954	CB	ALA	B	89	1068	1316	1311	-83	-19	-25	C
ATOM	5958	C	ALA	B	89	51.392	23.579	60.120	1.00	9.00		C
ANISOU	5958	C	ALA	B	89	1043	1138	1238	33	-31	-16	C
ATOM	5959	O	ALA	B	89	50.498	23.454	59.288	1.00	10.03		O
ANISOU	5959	O	ALA	B	89	1489	1303	1019	208	-1	-102	O
ATOM	5960	N	GLN	B	90	51.207	24.247	61.247	1.00	9.06		N
ANISOU	5960	N	GLN	B	90	1012	1281	1149	-7	-53	35	N
ATOM	5962	CA	GLN	B	90	49.923	24.907	61.453	1.00	9.73		C
ANISOU	5962	CA	GLN	B	90	1261	1141	1291	50	13	18	C
ATOM	5964	CB	GLN	B	90	49.785	25.542	62.825	1.00	10.40		C
ANISOU	5964	CB	GLN	B	90	1271	1419	1261	-57	-7	69	C
ATOM	5967	CG	GLN	B	90	49.780	24.593	63.941	1.00	12.85		C
ANISOU	5967	CG	GLN	B	90	1707	1528	1646	-59	0	117	C
ATOM	5970	CD	GLN	B	90	49.222	25.221	65.212	1.00	13.58		C
ANISOU	5970	CD	GLN	B	90	1782	1699	1678	105	71	62	C
ATOM	5971	OE1	GLN	B	90	49.616	26.332	65.569	1.00	13.60		O
ANISOU	5971	OE1	GLN	B	90	1934	1991	1242	183	25	-80	O
ATOM	5972	NE2	GLN	B	90	48.358	24.486	65.923	1.00	12.42		N
ANISOU	5972	NE2	GLN	B	90	1356	1676	1684	91	-38	-11	N
ATOM	5975	C	GLN	B	90	49.691	25.990	60.395	1.00	9.64		C
ANISOU	5975	C	GLN	B	90	1237	1207	1217	77	-7	6	C
ATOM	5976	O	GLN	B	90	48.554	26.433	60.235	1.00	9.52		O
ANISOU	5976	O	GLN	B	90	1004	1279	1332	230	32	10	O
ATOM	5977	N	ALA	B	91	50.731	26.415	59.695	1.00	8.47		N
ANISOU	5977	N	ALA	B	91	960	988	1268	125	62	36	N
ATOM	5979	CA	ALA	B	91	50.552	27.450	58.664	1.00	9.50		C
ANISOU	5979	CA	ALA	B	91	1061	1349	1199	2	132	73	C
ATOM	5981	CB	ALA	B	91	51.960	27.870	58.032	1.00	8.79		C
ANISOU	5981	CB	ALA	B	91	831	1234	1273	178	17	114	C
ATOM	5985	C	ALA	B	91	49.587	26.956	57.593	1.00	9.35		C
ANISOU	5985	C	ALA	B	91	1004	1353	1195	23	175	76	C
ATOM	5986	O	ALA	B	91	48.787	27.723	57.021	1.00	10.16		O
ANISOU	5986	O	ALA	B	91	1111	1516	1230	44	86	153	O
ATOM	5987	N	PHE	B	92	49.601	25.666	57.334	1.00	9.52		N
ANISOU	5987	N	PHE	B	92	906	1345	1363	23	99	67	N
ATOM	5989	CA	PHE	B	92	48.744	25.151	56.274	1.00	10.66		C
ANISOU	5989	CA	PHE	B	92	1235	1434	1381	-24	81	-2	C
ATOM	5991	CB	PHE	B	92	49.331	23.909	55.685	1.00	10.52		C
ANISOU	5991	CB	PHE	B	92	1237	1401	1358	22	-3	94	C
ATOM	5994	CG	PHE	B	92	50.669	24.168	55.106	1.00	11.85		C
ANISOU	5994	CG	PHE	B	92	1455	1571	1473	-91	16	-138	C
ATOM	5995	CD1	PHE	B	92	51.792	24.028	55.880	1.00	12.75		C
ANISOU	5995	CD1	PHE	B	92	1613	1740	1490	109	-116	75	C
ATOM	5997	CE1	PHE	B	92	52.984	24.348	55.392	1.00	13.45		C
ANISOU	5997	CE1	PHE	B	92	1713	1763	1633	91	-54	-182	C
ATOM	5999	CZ	PHE	B	92	53.123	24.896	54.120	1.00	13.04		C
ANISOU	5999	CZ	PHE	B	92	1657	1670	1627	158	90	-112	C
ATOM	6001	CE2	PHE	B	92	52.030	25.087	53.363	1.00	12.75		C
ANISOU	6001	CE2	PHE	B	92	1749	1517	1577	76	18	-27	C
ATOM	6003	CD2	PHE	B	92	50.785	24.731	53.862	1.00	10.07		C
ANISOU	6003	CD2	PHE	B	92	1330	1150	1346	36	-88	57	C
ATOM	6005	C	PHE	B	92	47.274	24.951	56.715	1.00	10.32		C
ANISOU	6005	C	PHE	B	92	1164	1372	1385	3	65	2	C
ATOM	6006	O	PHE	B	92	46.420	24.797	55.876	1.00	11.89		O

ANISOU	6006	O	PHE	B	92	1268	1712	1536	4	262	9	O
ATOM	6007	N	LEU	B	93	47.026	24.940	58.011	1.00	10.05		N
ANISOU	6007	N	LEU	B	93	1256	1274	1289	-26	35	-23	N
ATOM	6009	CA	LEU	B	93	45.694	24.731	58.538	1.00	11.00		C
ANISOU	6009	CA	LEU	B	93	1382	1446	1351	62	55	19	C
ATOM	6011	CB	LEU	B	93	45.726	23.953	59.873	1.00	11.63		C
ANISOU	6011	CB	LEU	B	93	1442	1573	1402	55	48	-21	C
ATOM	6014	CG	LEU	B	93	46.401	22.573	59.935	1.00	13.17		C
ANISOU	6014	CG	LEU	B	93	1626	1645	1733	-20	-49	12	C
ATOM	6016	CD1	LEU	B	93	46.303	21.974	61.335	1.00	15.24		C
ANISOU	6016	CD1	LEU	B	93	1834	1938	2018	3	12	-42	C
ATOM	6020	CD2	LEU	B	93	45.900	21.612	58.904	1.00	14.64		C
ANISOU	6020	CD2	LEU	B	93	1689	1917	1956	-108	187	-64	C
ATOM	6024	C	LEU	B	93	45.093	26.117	58.657	1.00	10.88		C
ANISOU	6024	C	LEU	B	93	1371	1426	1335	-4	64	52	C
ATOM	6025	O	LEU	B	93	43.991	26.376	58.160	1.00	10.87		O
ANISOU	6025	O	LEU	B	93	1181	1628	1319	-63	264	207	O
ATOM	6026	N	ILE	B	94	45.856	27.029	59.244	1.00	10.62		N
ANISOU	6026	N	ILE	B	94	1310	1358	1366	68	110	-19	N
ATOM	6028	CA	ILE	B	94	45.447	28.453	59.331	1.00	9.81		C
ANISOU	6028	CA	ILE	B	94	1222	1231	1273	85	-50	21	C
ATOM	6030	CB	ILE	B	94	46.467	29.249	60.086	1.00	9.86		C
ANISOU	6030	CB	ILE	B	94	1230	1248	1267	42	34	-11	C
ATOM	6032	CG1	ILE	B	94	46.521	28.794	61.545	1.00	9.26		C
ANISOU	6032	CG1	ILE	B	94	1150	1108	1259	48	57	0	C
ATOM	6035	CD1	ILE	B	94	47.680	29.341	62.241	1.00	10.93		C
ANISOU	6035	CD1	ILE	B	94	1540	1389	1223	63	-167	58	C
ATOM	6039	CG2	ILE	B	94	46.192	30.752	60.003	1.00	10.67		C
ANISOU	6039	CG2	ILE	B	94	1310	1358	1385	28	-244	36	C
ATOM	6043	C	ILE	B	94	45.230	29.044	57.942	1.00	8.96		C
ANISOU	6043	C	ILE	B	94	1128	1150	1125	77	-7	-53	C
ATOM	6044	O	ILE	B	94	44.209	29.739	57.708	1.00	7.40		O
ANISOU	6044	O	ILE	B	94	720	1160	929	220	-68	-225	O
ATOM	6045	N	GLY	B	95	46.110	28.688	57.029	1.00	8.38		N
ANISOU	6045	N	GLY	B	95	931	1124	1128	59	-104	-34	N
ATOM	6047	CA	GLY	B	95	46.096	29.181	55.671	1.00	8.42		C
ANISOU	6047	CA	GLY	B	95	1022	1014	1163	46	32	-5	C
ATOM	6050	C	GLY	B	95	45.349	28.347	54.643	1.00	8.32		C
ANISOU	6050	C	GLY	B	95	956	1039	1164	98	13	-31	C
ATOM	6051	O	GLY	B	95	45.515	28.594	53.469	1.00	7.83		O
ANISOU	6051	O	GLY	B	95	888	1020	1068	155	-152	-35	O
ATOM	6052	N	GLU	B	96	44.507	27.396	55.076	1.00	9.91		N
ANISOU	6052	N	GLU	B	96	1306	1180	1280	131	56	64	N
ATOM	6092	CE2	PHE	B	98	48.406	32.421	50.809	1.00	8.04		C
ANISOU	6092	CE2	PHE	B	98	873	1038	1141	-16	134	-53	C
ATOM	6094	CD2	PHE	B	98	47.329	31.833	51.489	1.00	7.22		C
ANISOU	6094	CD2	PHE	B	98	870	1059	813	-80	-116	-110	C
ATOM	6107	CD1	ILE	B	99	48.292	26.722	52.011	1.00	10.09		C
ANISOU	6107	CD1	ILE	B	99	1492	1202	1140	144	26	-113	C
ATOM	6180	N	ALA	B	105	54.005	28.271	49.038	1.00	9.13		N
ANISOU	6180	N	ALA	B	105	1049	1238	1181	70	-117	-132	N
ATOM	6182	CA	ALA	B	105	55.381	28.388	49.531	1.00	9.04		C
ANISOU	6182	CA	ALA	B	105	1060	1191	1183	18	-33	-63	C
ATOM	6184	CB	ALA	B	105	56.253	29.230	48.596	1.00	8.45		C
ANISOU	6184	CB	ALA	B	105	815	1231	1164	168	129	-103	C
ATOM	6188	C	ALA	B	105	55.306	28.999	50.919	1.00	9.68		C
ANISOU	6188	C	ALA	B	105	1123	1268	1285	99	-75	-94	C
ATOM	6189	O	ALA	B	105	54.538	29.894	51.166	1.00	10.56		O
ANISOU	6189	O	ALA	B	105	1437	1187	1385	419	-205	-179	O
ATOM	6190	N	LEU	B	106	56.079	28.436	51.826	1.00	8.73		N
ANISOU	6190	N	LEU	B	106	1185	1077	1054	77	-77	92	N

ATOM	6192	CA	LEU B 106	56.207	28.942	53.154	1.00	8.22		C
ANISOU	6192	CA	LEU B 106	999	1054	1069	42	15	15	C
ATOM	6194	CB	LEU B 106	55.882	27.798	54.109	1.00	8.63		C
ANISOU	6194	CB	LEU B 106	911	1341	1024	-121	-96	57	C
ATOM	6197	CG	LEU B 106	56.131	28.037	55.595	1.00	9.16		C
ANISOU	6197	CG	LEU B 106	1132	1223	1123	-100	23	-57	C
ATOM	6199	CD1	LEU B 106	55.385	29.180	56.142	1.00	8.85		C
ANISOU	6199	CD1	LEU B 106	553	1515	1292	118	142	157	C
ATOM	6203	CD2	LEU B 106	55.825	26.772	56.362	1.00	8.50		C
ANISOU	6203	CD2	LEU B 106	1056	1061	1110	90	-105	-32	C
ATOM	6207	C	LEU B 106	57.656	29.392	53.380	1.00	8.53		C
ANISOU	6207	C	LEU B 106	1094	1156	990	53	-5	8	C
ATOM	6208	O	LEU B 106	58.637	28.618	53.077	1.00	10.31		O
ANISOU	6208	O	LEU B 106	1389	1380	1146	200	-29	-35	O
ATOM	6209	N	VAL B 107	57.815	30.606	53.914	1.00	9.20		N
ANISOU	6209	N	VAL B 107	994	1227	1274	71	86	111	N
ATOM	6211	CA	VAL B 107	59.086	31.091	54.369	1.00	8.45		C
ANISOU	6211	CA	VAL B 107	1127	1016	1068	-5	-5	-44	C
ATOM	6213	CB	VAL B 107	59.669	32.219	53.447	1.00	8.09		C
ANISOU	6213	CB	VAL B 107	994	1167	913	3	66	14	C
ATOM	6215	CG1	VAL B 107	58.815	33.497	53.546	1.00	8.02		C
ANISOU	6215	CG1	VAL B 107	1117	933	994	-102	17	-30	C
ATOM	6219	CG2	VAL B 107	61.097	32.542	53.818	1.00	11.35		C
ANISOU	6219	CG2	VAL B 107	1411	1295	1603	92	-92	-64	C
ATOM	6223	C	VAL B 107	58.941	31.543	55.837	1.00	8.32		C
ANISOU	6223	C	VAL B 107	1038	1136	985	32	136	43	C
ATOM	6224	O	VAL B 107	57.908	32.086	56.284	1.00	7.58		O
ANISOU	6224	O	VAL B 107	883	1211	784	90	235	-140	O
ATOM	6225	N	LEU B 108	59.970	31.232	56.591	1.00	7.68		N
ANISOU	6225	N	LEU B 108	857	1075	983	70	85	33	N
ATOM	6227	CA	LEU B 108	60.051	31.596	58.009	1.00	8.53		C
ANISOU	6227	CA	LEU B 108	1135	1010	1094	15	-7	21	C
ATOM	6229	CB	LEU B 108	61.048	30.678	58.695	1.00	8.58		C
ANISOU	6229	CB	LEU B 108	1056	1185	1015	-6	2	86	C
ATOM	6232	CG	LEU B 108	60.618	29.207	58.633	1.00	8.97		C
ANISOU	6232	CG	LEU B 108	1156	1113	1139	137	20	-64	C
ATOM	6234	CD1	LEU B 108	61.423	28.389	59.594	1.00	10.92		C
ANISOU	6234	CD1	LEU B 108	1506	1291	1350	-97	-25	223	C
ATOM	6238	CD2	LEU B 108	59.183	28.999	58.920	1.00	13.97		C
ANISOU	6238	CD2	LEU B 108	1668	1709	1927	91	44	20	C
ATOM	6242	C	LEU B 108	60.467	33.038	58.193	1.00	9.21		C
ANISOU	6242	C	LEU B 108	1198	1096	1204	-18	9	37	C
ATOM	6243	O	LEU B 108	61.370	33.529	57.533	1.00	9.90		O
ANISOU	6243	O	LEU B 108	1292	1117	1350	-99	78	-6	O
ATOM	6244	N	GLY B 109	59.805	33.700	59.120	1.00	9.66		N
ANISOU	6244	N	GLY B 109	1258	1163	1247	-154	115	67	N
ATOM	6246	CA	GLY B 109	60.014	35.112	59.347	1.00	10.34		C
ANISOU	6246	CA	GLY B 109	1424	1195	1308	-48	76	-92	C
ATOM	6249	C	GLY B 109	61.409	35.594	59.786	1.00	10.72		C
ANISOU	6249	C	GLY B 109	1319	1301	1451	-33	84	35	C
ATOM	6250	O	GLY B 109	61.710	36.784	59.600	1.00	13.56		O
ANISOU	6250	O	GLY B 109	1777	1530	1845	-170	-1	117	O
ATOM	6251	N	ASP B 110	62.202	34.762	60.441	1.00	9.78		N
ANISOU	6251	N	ASP B 110	1274	1173	1266	-53	68	34	N
ATOM	6253	CA	ASP B 110	63.532	35.128	60.905	1.00	9.40		C
ANISOU	6253	CA	ASP B 110	1233	1091	1247	-58	95	-20	C
ATOM	6255	CB	ASP B 110	63.814	34.749	62.362	1.00	9.23		C
ANISOU	6255	CB	ASP B 110	1075	1074	1356	-71	-21	56	C
ATOM	6258	CG	ASP B 110	63.702	33.203	62.666	1.00	12.59		C
ANISOU	6258	CG	ASP B 110	1778	1345	1659	-117	-82	89	C
ATOM	6259	OD1	ASP B 110	63.453	32.382	61.753	1.00	14.33		O

ANISOU	6259	OD1	ASP	B	110	2035	1474	1934	117	172	118	O
ATOM	6260	OD2	ASP	B	110	63.825	32.741	63.839	1.00	15.01		O
ANISOU	6260	OD2	ASP	B	110	2374	1602	1726	-207	-54	59	O
ATOM	6261	C	ASP	B	110	64.597	34.525	60.028	1.00	10.65		C
ANISOU	6261	C	ASP	B	110	1379	1253	1415	53	-9	21	C
ATOM	6262	O	ASP	B	110	65.683	34.434	60.466	1.00	11.23		O
ANISOU	6262	O	ASP	B	110	1206	1486	1576	-27	71	-122	O
ATOM	6263	N	ASN	B	111	64.262	34.072	58.820	1.00	9.85		N
ANISOU	6263	N	ASN	B	111	1376	1111	1254	-57	9	-39	N
ATOM	6265	CA	ASN	B	111	65.297	33.533	57.911	1.00	9.92		C
ANISOU	6265	CA	ASN	B	111	1204	1250	1312	25	-29	36	C
ATOM	6267	CB	ASN	B	111	64.813	32.270	57.170	1.00	10.67		C
ANISOU	6267	CB	ASN	B	111	1299	1417	1336	-10	-72	-53	C
ATOM	6270	CG	ASN	B	111	64.890	30.962	57.979	1.00	11.50		C
ANISOU	6270	CG	ASN	B	111	1509	1450	1410	77	-37	-9	C
ATOM	6271	OD1	ASN	B	111	65.146	29.946	57.368	1.00	11.48		O
ANISOU	6271	OD1	ASN	B	111	1002	1601	1757	97	-33	-236	O
ATOM	6272	ND2	ASN	B	111	64.595	30.956	59.302	1.00	9.14		N
ANISOU	6272	ND2	ASN	B	111	729	1293	1450	238	201	-153	N
ATOM	6275	C	ASN	B	111	65.711	34.553	56.868	1.00	10.47		C
ANISOU	6275	C	ASN	B	111	1218	1426	1332	6	79	14	C
ATOM	6276	O	ASN	B	111	64.878	35.123	56.158	1.00	11.11		O
ANISOU	6276	O	ASN	B	111	1014	1732	1475	93	345	93	O
ATOM	6277	N	LEU	B	112	67.018	34.729	56.725	1.00	8.72		N
ANISOU	6277	N	LEU	B	112	957	1229	1127	103	8	5	N
ATOM	6279	CA	LEU	B	112	67.577	35.716	55.835	1.00	10.72		C
ANISOU	6279	CA	LEU	B	112	1322	1374	1377	58	35	-22	C
ATOM	6281	CB	LEU	B	112	68.444	36.698	56.657	1.00	10.59		C
ANISOU	6281	CB	LEU	B	112	1213	1348	1460	62	-92	-33	C
ATOM	6284	CG	LEU	B	112	68.836	37.998	55.916	1.00	15.52		C
ANISOU	6284	CG	LEU	B	112	2092	1879	1925	-24	-53	-7	C
ATOM	6286	CD1	LEU	B	112	69.423	39.166	56.816	1.00	16.60		C
ANISOU	6286	CD1	LEU	B	112	2240	1995	2071	-51	-172	-15	C
ATOM	6290	CD2	LEU	B	112	69.775	37.779	54.873	1.00	17.98		C
ANISOU	6290	CD2	LEU	B	112	2259	2301	2271	-1	76	-163	C
ATOM	6294	C	LEU	B	112	68.475	34.973	54.827	1.00	9.88		C
ANISOU	6294	C	LEU	B	112	1175	1368	1209	75	80	2	C
ATOM	6295	O	LEU	B	112	69.411	34.350	55.217	1.00	11.66		O
ANISOU	6295	O	LEU	B	112	1490	1423	1514	112	11	82	O
ATOM	6296	N	TYR	B	113	68.162	35.030	53.563	1.00	9.61		N
ANISOU	6296	N	TYR	B	113	1127	1258	1266	59	42	-9	N
ATOM	6298	CA	TYR	B	113	68.953	34.395	52.503	1.00	7.80		C
ANISOU	6298	CA	TYR	B	113	999	1040	923	4	94	26	C
ATOM	6300	CB	TYR	B	113	68.065	33.564	51.581	1.00	7.86		C
ANISOU	6300	CB	TYR	B	113	1027	1071	886	7	152	26	C
ATOM	6303	CG	TYR	B	113	67.339	32.444	52.224	1.00	9.60		C
ANISOU	6303	CG	TYR	B	113	1325	1269	1053	-43	-63	29	C
ATOM	6304	CD1	TYR	B	113	66.069	32.627	52.749	1.00	11.51		C
ANISOU	6304	CD1	TYR	B	113	1341	1555	1476	-4	99	21	C
ATOM	6306	CE1	TYR	B	113	65.378	31.548	53.357	1.00	10.21		C
ANISOU	6306	CE1	TYR	B	113	1180	1285	1413	23	46	8	C
ATOM	6308	CZ	TYR	B	113	65.973	30.311	53.427	1.00	11.84		C
ANISOU	6308	CZ	TYR	B	113	1573	1440	1484	-3	84	54	C
ATOM	6309	OH	TYR	B	113	65.307	29.256	54.015	1.00	10.12		O
ANISOU	6309	OH	TYR	B	113	946	1215	1681	158	-103	326	O
ATOM	6311	CE2	TYR	B	113	67.183	30.109	52.837	1.00	11.43		C
ANISOU	6311	CE2	TYR	B	113	1157	1317	1868	72	-151	158	C
ATOM	6313	CD2	TYR	B	113	67.860	31.177	52.211	1.00	10.78		C
ANISOU	6313	CD2	TYR	B	113	1431	1394	1271	115	-249	126	C
ATOM	6315	C	TYR	B	113	69.639	35.484	51.642	1.00	7.73		C
ANISOU	6315	C	TYR	B	113	1030	1027	878	43	56	33	C

ATOM	6316	O	TYR	B	113	69.122	36.576	51.488	1.00	7.43		O
ANISOU	6316	O	TYR	B	113	1163	1019	639	56	111	197	O
ATOM	6317	N	TYR	B	114	70.843	35.209	51.135	1.00	7.30		N
ANISOU	6317	N	TYR	B	114	1038	916	817	78	37	-24	N
ATOM	6319	CA	TYR	B	114	71.408	36.134	50.234	1.00	7.79		C
ANISOU	6319	CA	TYR	B	114	882	1085	990	69	20	22	C
ATOM	6321	CB	TYR	B	114	72.075	37.313	50.967	1.00	8.84		C
ANISOU	6321	CB	TYR	B	114	1069	1172	1115	76	64	44	C
ATOM	6383	CD1	PHE	B	118	68.327	32.317	47.151	1.00	11.71		C
ANISOU	6383	CD1	PHE	B	118	1659	1400	1388	23	178	61	C
ATOM	6385	CE1	PHE	B	118	67.478	31.934	48.165	1.00	10.86		C
ANISOU	6385	CE1	PHE	B	118	1297	1145	1683	-313	161	-107	C
ATOM	6387	CZ	PHE	B	118	66.568	32.812	48.671	1.00	11.10		C
ANISOU	6387	CZ	PHE	B	118	1255	1529	1430	-14	159	112	C
ATOM	6389	CE2	PHE	B	118	66.565	34.096	48.281	1.00	8.70		C
ANISOU	6389	CE2	PHE	B	118	957	1364	982	81	60	-100	C
ATOM	6391	CD2	PHE	B	118	67.419	34.500	47.291	1.00	10.35		C
ANISOU	6391	CD2	PHE	B	118	951	1393	1588	-123	128	124	C
ATOM	6441	CD2	LEU	B	121	68.933	28.316	46.002	1.00	14.06		C
ANISOU	6441	CD2	LEU	B	121	1921	1916	1505	9	196	85	C
ATOM	6460	CD2	LEU	B	122	63.707	31.467	46.720	1.00	9.31		C
ANISOU	6460	CD2	LEU	B	122	1313	1116	1108	-102	70	113	C
ATOM	6586	CA	ALA	B	132	57.759	19.555	47.596	1.00	7.62		C
ANISOU	6586	CA	ALA	B	132	1079	829	987	20	6	-63	C
ATOM	6588	CB	ALA	B	132	57.651	19.081	48.995	1.00	7.68		C
ANISOU	6588	CB	ALA	B	132	999	839	1077	-14	-149	-79	C
ATOM	6592	C	ALA	B	132	59.193	19.811	47.242	1.00	7.81		C
ANISOU	6592	C	ALA	B	132	1048	937	982	-1	-135	-92	C
ATOM	6593	O	ALA	B	132	59.901	18.907	46.753	1.00	9.52		O
ANISOU	6593	O	ALA	B	132	1201	1199	1213	-23	-45	-180	O
ATOM	6594	N	SER	B	133	59.624	21.054	47.457	1.00	7.96		N
ANISOU	6594	N	SER	B	133	1120	955	946	4	24	57	N
ATOM	6596	CA	SER	B	133	61.003	21.436	47.325	1.00	7.43		C
ANISOU	6596	CA	SER	B	133	863	1003	957	13	-60	-44	C
ATOM	6598	CB	SER	B	133	61.254	22.334	46.130	1.00	7.20		C
ANISOU	6598	CB	SER	B	133	722	952	1061	9	-42	-6	C
ATOM	6603	C	SER	B	133	61.483	22.145	48.596	1.00	7.62		C
ANISOU	6603	C	SER	B	133	986	957	950	14	48	-40	C
ATOM	6604	O	SER	B	133	60.831	23.068	49.081	1.00	8.09		O
ANISOU	6604	O	SER	B	133	941	1173	958	-58	192	-139	O
ATOM	6605	N	VAL	B	134	62.653	21.739	49.068	1.00	6.84		N
ANISOU	6605	N	VAL	B	134	804	875	916	48	102	-104	N
ATOM	6607	CA	VAL	B	134	63.297	22.261	50.256	1.00	6.93		C
ANISOU	6607	CA	VAL	B	134	868	930	834	19	-8	-46	C
ATOM	6609	CB	VAL	B	134	63.078	21.349	51.462	1.00	8.11		C
ANISOU	6609	CB	VAL	B	134	1060	1036	985	-19	65	-54	C
ATOM	6611	CG1	VAL	B	134	61.631	21.151	51.670	1.00	8.90		C
ANISOU	6611	CG1	VAL	B	134	1228	1338	814	-69	-51	20	C
ATOM	6615	CG2	VAL	B	134	63.850	20.005	51.357	1.00	9.68		C
ANISOU	6615	CG2	VAL	B	134	1360	1156	1158	-123	20	12	C
ATOM	6619	C	VAL	B	134	64.797	22.369	49.946	1.00	7.97		C
ANISOU	6619	C	VAL	B	134	995	1003	1027	-43	0	-43	C
ATOM	6620	O	VAL	B	134	65.247	21.827	48.978	1.00	9.70		O
ANISOU	6620	O	VAL	B	134	1066	1341	1278	-36	-109	-156	O
ATOM	6621	N	PHE	B	135	65.546	23.086	50.772	1.00	7.57		N
ANISOU	6621	N	PHE	B	135	1017	1087	770	15	-49	-23	N
ATOM	6623	CA	PHE	B	135	66.943	23.426	50.530	1.00	8.09		C
ANISOU	6623	CA	PHE	B	135	1012	1097	963	73	-29	1	C
ATOM	6625	CB	PHE	B	135	67.060	24.916	50.305	1.00	8.70		C
ANISOU	6625	CB	PHE	B	135	832	1327	1146	-61	51	-8	C
ATOM	6628	CG	PHE	B	135	66.273	25.377	49.135	1.00	10.94		C

ANISOU	6628	CG	PHE	B	135	1378	1321	1455	-61	-99	-36	C
ATOM	6629	CD1	PHE	B	135	64.942	25.787	49.294	1.00	14.22		C
ANISOU	6629	CD1	PHE	B	135	1604	1903	1893	17	3	-14	C
ATOM	6631	CE1	PHE	B	135	64.203	26.127	48.196	1.00	16.39		C
ANISOU	6631	CE1	PHE	B	135	1777	2233	2218	141	77	76	C
ATOM	6633	CZ	PHE	B	135	64.778	26.094	46.936	1.00	17.11		C
ANISOU	6633	CZ	PHE	B	135	2309	2123	2068	20	-158	43	C
ATOM	6635	CE2	PHE	B	135	66.033	25.682	46.784	1.00	15.86		C
ANISOU	6635	CE2	PHE	B	135	2082	2010	1932	-51	76	89	C
ATOM	6637	CD2	PHE	B	135	66.787	25.306	47.883	1.00	14.39		C
ANISOU	6637	CD2	PHE	B	135	1818	1885	1763	-16	78	51	C
ATOM	6639	C	PHE	B	135	67.798	22.981	51.711	1.00	8.70		C
ANISOU	6639	C	PHE	B	135	1170	1129	1004	46	-36	-35	C
ATOM	6640	O	PHE	B	135	67.394	23.171	52.873	1.00	9.72		O
ANISOU	6640	O	PHE	B	135	1520	1230	940	-29	-39	247	O
ATOM	6641	N	ALA	B	136	68.910	22.321	51.386	1.00	7.74		N
ANISOU	6641	N	ALA	B	136	892	1086	961	-16	-61	100	N
ATOM	6643	CA	ALA	B	136	69.870	21.847	52.388	1.00	7.69		C
ANISOU	6643	CA	ALA	B	136	965	998	958	-3	-41	84	C
ATOM	6645	CB	ALA	B	136	70.215	20.419	52.076	1.00	8.30		C
ANISOU	6645	CB	ALA	B	136	970	1226	956	17	-65	41	C
ATOM	6649	C	ALA	B	136	71.120	22.726	52.405	1.00	8.69		C
ANISOU	6649	C	ALA	B	136	1163	1108	1030	-9	-2	55	C
ATOM	6650	O	ALA	B	136	71.699	23.024	51.348	1.00	9.88		O
ANISOU	6650	O	ALA	B	136	1248	1395	1108	-236	212	50	O
ATOM	6651	N	TYR	B	137	71.562	23.103	53.600	1.00	7.61		N
ANISOU	6651	N	TYR	B	137	1117	1021	750	-86	47	79	N
ATOM	6653	CA	TYR	B	137	72.668	24.023	53.761	1.00	7.01		C
ANISOU	6653	CA	TYR	B	137	858	959	848	50	-29	4	C
ATOM	6655	CB	TYR	B	137	72.170	25.396	54.039	1.00	5.60		C
ANISOU	6655	CB	TYR	B	137	660	986	481	158	64	-15	C
ATOM	6658	CG	TYR	B	137	73.094	26.593	54.050	1.00	7.74		C
ANISOU	6658	CG	TYR	B	137	972	916	1050	145	-45	29	C
ATOM	6659	CD1	TYR	B	137	73.395	27.309	52.887	1.00	8.47		C
ANISOU	6659	CD1	TYR	B	137	1084	1200	931	-20	-28	-89	C
ATOM	6661	CE1	TYR	B	137	74.172	28.474	52.929	1.00	8.41		C
ANISOU	6661	CE1	TYR	B	137	1046	1076	1072	-32	10	87	C
ATOM	6663	CZ	TYR	B	137	74.671	28.944	54.149	1.00	7.72		C
ANISOU	6663	CZ	TYR	B	137	958	897	1076	-37	91	87	C
ATOM	6664	OH	TYR	B	137	75.410	30.080	54.226	1.00	8.42		O
ANISOU	6664	OH	TYR	B	137	896	941	1359	-155	38	-107	O
ATOM	6666	CE2	TYR	B	137	74.379	28.295	55.304	1.00	5.35		C
ANISOU	6666	CE2	TYR	B	137	523	792	718	208	-123	159	C
ATOM	6668	CD2	TYR	B	137	73.603	27.079	55.236	1.00	9.47		C
ANISOU	6668	CD2	TYR	B	137	1184	1225	1189	64	50	-110	C
ATOM	6670	C	TYR	B	137	73.600	23.560	54.864	1.00	6.91		C
ANISOU	6670	C	TYR	B	137	996	881	748	-6	-54	13	C
ATOM	6671	O	TYR	B	137	73.138	23.215	55.943	1.00	6.59		O
ANISOU	6671	O	TYR	B	137	916	777	810	-72	-25	-82	O
ATOM	6672	N	HIS	B	138	74.892	23.489	54.518	1.00	5.78		N
ANISOU	6672	N	HIS	B	138	761	682	750	-84	0	46	N
ATOM	6674	CA	HIS	B	138	75.898	23.030	55.456	1.00	7.38		C
ANISOU	6674	CA	HIS	B	138	962	860	980	-117	5	13	C
ATOM	6676	CB	HIS	B	138	77.239	22.816	54.766	1.00	7.04		C
ANISOU	6676	CB	HIS	B	138	882	754	1038	-86	-53	-59	C
ATOM	6679	CG	HIS	B	138	78.208	22.038	55.560	1.00	7.62		C
ANISOU	6679	CG	HIS	B	138	1045	1008	841	-85	77	5	C
ATOM	6680	ND1	HIS	B	138	78.874	22.569	56.641	1.00	7.25		N
ANISOU	6680	ND1	HIS	B	138	698	1154	899	-97	-265	16	N
ATOM	6682	CE1	HIS	B	138	79.689	21.641	57.134	1.00	10.52		C
ANISOU	6682	CE1	HIS	B	138	1577	1323	1097	46	-34	-95	C

ATOM	6684	NE2	HIS	B	138	79.591	20.553	56.399	1.00	10.01		N
ANISOU	6684	NE2	HIS	B	138	1385	938	1480	-44	-5	188	N
ATOM	6686	CD2	HIS	B	138	78.593	20.739	55.476	1.00	10.19		C
ANISOU	6686	CD2	HIS	B	138	1297	1127	1448	-135	-63	-16	C
ATOM	6688	C	HIS	B	138	76.043	24.035	56.579	1.00	8.16		C
ANISOU	6688	C	HIS	B	138	1013	976	1110	-39	-35	-7	C
ATOM	6689	O	HIS	B	138	76.275	25.202	56.340	1.00	7.93		O
ANISOU	6689	O	HIS	B	138	956	838	1216	-142	0	-97	O
ATOM	6690	N	VAL	B	139	75.977	23.554	57.798	1.00	8.34		N
ANISOU	6690	N	VAL	B	139	1028	1039	1098	-196	33	20	N
ATOM	6692	CA	VAL	B	139	76.073	24.411	58.971	1.00	9.44		C
ANISOU	6692	CA	VAL	B	139	1208	1219	1160	-37	-4	-24	C
ATOM	6694	CB	VAL	B	139	74.667	24.696	59.635	1.00	9.21		C
ANISOU	6694	CB	VAL	B	139	1168	1183	1148	-35	-58	6	C
ATOM	6696	CG1	VAL	B	139	73.811	25.510	58.743	1.00	11.13		C
ANISOU	6696	CG1	VAL	B	139	1331	1479	1419	68	18	24	C
ATOM	6700	CG2	VAL	B	139	73.947	23.396	60.109	1.00	11.01		C
ANISOU	6700	CG2	VAL	B	139	1348	1453	1381	-95	-62	-29	C
ATOM	6704	C	VAL	B	139	76.985	23.839	60.033	1.00	9.80		C
ANISOU	6704	C	VAL	B	139	1299	1255	1168	-39	-23	-4	C
ATOM	6705	O	VAL	B	139	77.306	22.617	60.057	1.00	9.37		O
ANISOU	6705	O	VAL	B	139	1305	1253	1001	1	-149	-156	O
ATOM	6706	N	LEU	B	140	77.391	24.727	60.951	1.00	10.87		N
ANISOU	6706	N	LEU	B	140	1521	1324	1284	-31	-91	-36	N
ATOM	6708	CA	LEU	B	140	78.219	24.302	62.084	1.00	12.83		C
ANISOU	6708	CA	LEU	B	140	1660	1567	1646	-34	-118	-38	C
ATOM	6710	CB	LEU	B	140	78.877	25.529	62.771	1.00	12.37		C
ANISOU	6710	CB	LEU	B	140	1653	1531	1516	-59	-36	-81	C
ATOM	6713	CG	LEU	B	140	79.758	25.214	63.970	1.00	14.74		C
ANISOU	6713	CG	LEU	B	140	1823	1899	1878	-54	-73	-27	C
ATOM	6723	C	LEU	B	140	77.442	23.534	63.146	1.00	12.95		C
ANISOU	6723	C	LEU	B	140	1726	1589	1605	-97	-60	-64	C
ATOM	6724	O	LEU	B	140	77.970	22.606	63.760	1.00	13.82		O
ANISOU	6724	O	LEU	B	140	1831	1470	1950	-154	-75	-39	O
ATOM	6725	N	ASP	B	141	76.194	23.896	63.387	1.00	13.93		N
ANISOU	6725	N	ASP	B	141	1874	1734	1681	-43	-86	-59	N
ATOM	6727	CA	ASP	B	141	75.470	23.282	64.525	1.00	15.67		C
ANISOU	6727	CA	ASP	B	141	2062	1924	1967	-90	2	-33	C
ATOM	6729	CB	ASP	B	141	75.302	24.274	65.696	1.00	17.30		C
ANISOU	6729	CB	ASP	B	141	2319	2077	2178	-72	124	-46	C
ATOM	6732	CG	ASP	B	141	76.599	24.454	66.503	1.00	24.35		C
ANISOU	6732	CG	ASP	B	141	3033	3149	3069	-11	-121	-112	C
ATOM	6733	OD1	ASP	B	141	77.173	23.463	67.054	1.00	32.27		O
ANISOU	6733	OD1	ASP	B	141	4384	3728	4149	95	-202	131	O
ATOM	6734	OD2	ASP	B	141	77.141	25.578	66.674	1.00	31.32		O
ANISOU	6734	OD2	ASP	B	141	4010	3615	4273	-215	58	4	O
ATOM	6735	C	ASP	B	141	74.147	22.745	64.074	1.00	14.19		C
ANISOU	6735	C	ASP	B	141	1877	1773	1740	-22	4	-46	C
ATOM	6736	O	ASP	B	141	73.111	23.353	64.319	1.00	13.16		O
ANISOU	6736	O	ASP	B	141	1857	1656	1485	-151	119	-190	O
ATOM	6737	N	PRO	B	142	74.204	21.641	63.323	1.00	11.98		N
ANISOU	6737	N	PRO	B	142	1663	1461	1427	-104	-9	41	N
ATOM	6738	CA	PRO	B	142	73.001	21.052	62.757	1.00	12.35		C
ANISOU	6738	CA	PRO	B	142	1605	1606	1481	-32	29	8	C
ATOM	6740	CB	PRO	B	142	73.512	19.793	62.055	1.00	11.69		C
ANISOU	6740	CB	PRO	B	142	1607	1437	1396	-23	18	55	C
ATOM	6743	CG	PRO	B	142	74.815	19.540	62.654	1.00	12.24		C
ANISOU	6743	CG	PRO	B	142	1565	1680	1405	-127	59	-50	C
ATOM	6746	CD	PRO	B	142	75.392	20.910	62.912	1.00	11.54		C
ANISOU	6746	CD	PRO	B	142	1700	1419	1266	-118	-11	73	C
ATOM	6749	C	PRO	B	142	71.975	20.655	63.784	1.00	11.48		C

ANISOU	6749	C	PRO	B	142	1499	1453	1407	-56	17	59	C
ATOM	6750	O	PRO	B	142	70.808	20.638	63.428	1.00	10.15		O
ANISOU	6750	O	PRO	B	142	1309	1330	1217	-391	-64	-1	O
ATOM	6751	N	GLU	B	143	72.388	20.420	65.023	1.00	11.54		N
ANISOU	6751	N	GLU	B	143	1489	1424	1468	-60	-53	-3	N
ATOM	6753	CA	GLU	B	143	71.448	19.994	66.049	1.00	12.07		C
ANISOU	6753	CA	GLU	B	143	1511	1628	1444	-36	-31	-22	C
ATOM	6755	CB	GLU	B	143	72.171	19.637	67.344	1.00	13.79		C
ANISOU	6755	CB	GLU	B	143	1681	1859	1697	8	49	45	C
ATOM	6758	CG	GLU	B	143	72.826	20.830	67.981	1.00	15.76		C
ANISOU	6758	CG	GLU	B	143	1904	1976	2105	-85	-15	-94	C
ATOM	6761	CD	GLU	B	143	74.214	21.089	67.405	1.00	20.30		C
ANISOU	6761	CD	GLU	B	143	2408	2669	2634	-17	149	13	C
ATOM	6762	OE1	GLU	B	143	74.563	20.444	66.395	1.00	19.55		O
ANISOU	6762	OE1	GLU	B	143	2313	2810	2302	-99	102	87	O
ATOM	6763	OE2	GLU	B	143	74.965	21.903	68.001	1.00	24.75		O
ANISOU	6763	OE2	GLU	B	143	3186	3145	3070	-179	-74	-125	O
ATOM	6764	C	GLU	B	143	70.333	21.009	66.336	1.00	11.68		C
ANISOU	6764	C	GLU	B	143	1624	1457	1354	-44	-30	-53	C
ATOM	6765	O	GLU	B	143	69.352	20.696	66.979	1.00	9.73		O
ANISOU	6765	O	GLU	B	143	1545	1214	936	-107	33	-65	O
ATOM	6766	N	ARG	B	144	70.506	22.240	65.885	1.00	11.97		N
ANISOU	6766	N	ARG	B	144	1794	1593	1160	-36	-19	12	N
ATOM	6768	CA	ARG	B	144	69.509	23.266	66.093	1.00	13.45		C
ANISOU	6768	CA	ARG	B	144	1837	1674	1598	21	-7	37	C
ATOM	6770	CB	ARG	B	144	70.237	24.620	66.071	1.00	15.47		C
ANISOU	6770	CB	ARG	B	144	2137	1886	1855	-1	-38	12	C
ATOM	6773	CG	ARG	B	144	71.340	24.811	67.084	1.00	20.14		C
ANISOU	6773	CG	ARG	B	144	2561	2496	2593	106	-246	-9	C
ATOM	6776	CD	ARG	B	144	72.001	26.227	67.029	1.00	26.90		C
ANISOU	6776	CD	ARG	B	144	3436	3168	3615	-168	-13	63	C
ATOM	6779	NE	ARG	B	144	70.949	27.241	66.875	1.00	31.34		N
ANISOU	6779	NE	ARG	B	144	3967	3791	4149	61	45	97	N
ATOM	6781	CZ	ARG	B	144	70.986	28.287	66.036	1.00	34.22		C
ANISOU	6781	CZ	ARG	B	144	4475	4169	4355	9	73	125	C
ATOM	6782	NH1	ARG	B	144	72.075	28.538	65.266	1.00	32.27		N
ANISOU	6782	NH1	ARG	B	144	4122	3897	4241	-20	78	-1	N
ATOM	6785	NH2	ARG	B	144	69.914	29.089	65.990	1.00	35.63		N
ANISOU	6785	NH2	ARG	B	144	4451	4576	4507	116	108	154	N
ATOM	6788	C	ARG	B	144	68.412	23.304	65.043	1.00	12.87		C
ANISOU	6788	C	ARG	B	144	1792	1596	1503	54	69	42	C
ATOM	6789	O	ARG	B	144	67.444	24.101	65.135	1.00	14.97		O
ANISOU	6789	O	ARG	B	144	2246	1672	1768	257	82	-29	O
ATOM	6790	N	TYR	B	145	68.517	22.441	64.053	1.00	10.68		N
ANISOU	6790	N	TYR	B	145	1475	1237	1344	97	86	31	N
ATOM	6792	CA	TYR	B	145	67.695	22.533	62.849	1.00	10.53		C
ANISOU	6792	CA	TYR	B	145	1291	1382	1329	67	142	-3	C
ATOM	6794	CB	TYR	B	145	68.608	23.026	61.691	1.00	10.83		C
ANISOU	6794	CB	TYR	B	145	1355	1359	1401	-27	114	12	C
ATOM	6797	CG	TYR	B	145	69.032	24.421	61.933	1.00	13.77		C
ANISOU	6797	CG	TYR	B	145	1780	1785	1666	0	58	-15	C
ATOM	6798	CD1	TYR	B	145	70.318	24.714	62.163	1.00	15.65		C
ANISOU	6798	CD1	TYR	B	145	1875	2174	1895	-218	42	-129	C
ATOM	6800	CE1	TYR	B	145	70.727	26.016	62.414	1.00	17.91		C
ANISOU	6800	CE1	TYR	B	145	2408	2055	2342	32	209	-73	C
ATOM	6802	CZ	TYR	B	145	69.822	26.981	62.510	1.00	17.56		C
ANISOU	6802	CZ	TYR	B	145	2159	2294	2219	32	-96	246	C
ATOM	6803	OH	TYR	B	145	70.229	28.234	62.824	1.00	21.30		O
ANISOU	6803	OH	TYR	B	145	2441	2613	3036	-86	99	-8	O
ATOM	6805	CE2	TYR	B	145	68.491	26.723	62.290	1.00	19.02		C
ANISOU	6805	CE2	TYR	B	145	2303	2422	2501	-201	155	9	C

ATOM	6807	CD2	TYR	B	145	68.102	25.442	62.016	1.00	15.32		C
ANISOU	6807	CD2	TYR	B	145	1943	1976	1900	74	64	-151	C
ATOM	6809	C	TYR	B	145	67.086	21.207	62.443	1.00	9.80		C
ANISOU	6809	C	TYR	B	145	1172	1346	1205	45	109	-12	C
ATOM	6810	O	TYR	B	145	67.382	20.153	63.035	1.00	10.36		O
ANISOU	6810	O	TYR	B	145	1113	1496	1327	55	82	22	O
ATOM	6811	N	GLY	B	146	66.245	21.252	61.416	1.00	9.51		N
ANISOU	6811	N	GLY	B	146	1090	1219	1303	92	46	97	N
ATOM	6813	CA	GLY	B	146	65.809	20.060	60.725	1.00	9.04		C
ANISOU	6813	CA	GLY	B	146	1118	1194	1122	125	8	93	C
ATOM	6816	C	GLY	B	146	67.071	19.588	59.985	1.00	8.91		C
ANISOU	6816	C	GLY	B	146	1065	1171	1148	34	55	97	C
ATOM	6817	O	GLY	B	146	67.770	20.401	59.397	1.00	9.39		O
ANISOU	6817	O	GLY	B	146	1321	1071	1173	69	8	247	O
ATOM	6818	N	VAL	B	147	67.379	18.303	60.031	1.00	7.72		N
ANISOU	6818	N	VAL	B	147	910	1078	945	-43	34	53	N
ATOM	6820	CA	VAL	B	147	68.588	17.797	59.425	1.00	7.79		C
ANISOU	6820	CA	VAL	B	147	1082	909	965	46	25	110	C
ATOM	6822	CB	VAL	B	147	69.524	17.185	60.489	1.00	7.20		C
ANISOU	6822	CB	VAL	B	147	805	998	933	-24	-110	-105	C
ATOM	6824	CG1	VAL	B	147	70.794	16.587	59.878	1.00	6.99		C
ANISOU	6824	CG1	VAL	B	147	830	821	1005	-368	69	34	C
ATOM	6828	CG2	VAL	B	147	69.781	18.169	61.548	1.00	8.39		C
ANISOU	6828	CG2	VAL	B	147	1018	1013	1155	135	-216	-53	C
ATOM	6832	C	VAL	B	147	68.245	16.725	58.381	1.00	8.38		C
ANISOU	6832	C	VAL	B	147	1009	1190	983	-30	-97	50	C
ATOM	6833	O	VAL	B	147	67.457	15.811	58.627	1.00	9.14		O
ANISOU	6833	O	VAL	B	147	1233	1203	1036	9	9	118	O
ATOM	6834	N	VAL	B	148	68.871	16.843	57.216	1.00	7.84		N
ANISOU	6834	N	VAL	B	148	792	1137	1050	10	20	88	N
ATOM	6836	CA	VAL	B	148	68.695	15.888	56.162	1.00	8.13		C
ANISOU	6836	CA	VAL	B	148	958	1123	1006	27	-4	47	C
ATOM	6838	CB	VAL	B	148	68.232	16.534	54.839	1.00	8.35		C
ANISOU	6838	CB	VAL	B	148	1031	1112	1027	41	-40	28	C
ATOM	6840	CG1	VAL	B	148	69.264	17.584	54.296	1.00	9.93		C
ANISOU	6840	CG1	VAL	B	148	1371	1201	1197	0	-119	-2	C
ATOM	6844	CG2	VAL	B	148	67.975	15.422	53.760	1.00	9.54		C
ANISOU	6844	CG2	VAL	B	148	1275	1213	1135	87	-49	118	C
ATOM	6848	C	VAL	B	148	69.972	15.066	55.962	1.00	8.79		C
ANISOU	6848	C	VAL	B	148	1135	1173	1030	20	0	-24	C
ATOM	6849	O	VAL	B	148	71.100	15.607	55.875	1.00	8.58		O
ANISOU	6849	O	VAL	B	148	977	1237	1042	99	-62	-43	O
ATOM	6850	N	GLU	B	149	69.769	13.761	55.881	1.00	8.38		N
ANISOU	6850	N	GLU	B	149	1104	1038	1039	33	-84	48	N
ATOM	6852	CA	GLU	B	149	70.837	12.781	55.604	1.00	8.67		C
ANISOU	6852	CA	GLU	B	149	1179	1126	990	82	81	2	C
ATOM	6854	CB	GLU	B	149	70.701	11.584	56.570	1.00	8.74		C
ANISOU	6854	CB	GLU	B	149	1350	1044	924	70	62	55	C
ATOM	6863	C	GLU	B	149	70.737	12.254	54.186	1.00	7.88		C
ANISOU	6863	C	GLU	B	149	1057	937	998	34	39	-6	C
ATOM	6864	O	GLU	B	149	69.651	12.080	53.659	1.00	7.98		O
ANISOU	6864	O	GLU	B	149	866	976	1186	139	238	-174	O
ATOM	6873	CD1	PHE	B	150	72.557	14.895	52.134	1.00	12.11		C
ANISOU	6873	CD1	PHE	B	150	1643	1428	1531	22	-203	54	C
ATOM	6875	CE1	PHE	B	150	72.003	16.216	52.140	1.00	10.64		C
ANISOU	6875	CE1	PHE	B	150	1351	1173	1516	-115	-139	-97	C
ATOM	6877	CZ	PHE	B	150	71.046	16.534	51.256	1.00	10.18		C
ANISOU	6877	CZ	PHE	B	150	1334	1242	1290	-130	40	-33	C
ATOM	6879	CE2	PHE	B	150	70.623	15.549	50.351	1.00	11.13		C
ANISOU	6879	CE2	PHE	B	150	1491	1469	1268	38	-131	-124	C
ATOM	6881	CD2	PHE	B	150	71.171	14.282	50.341	1.00	10.74		C

ANISOU	6881	CD2	PHE	B	150	1347	1344	1386	-85	-161	29	C
ATOM	6952	CA	ALA	B	156	68.012	12.259	50.637	1.00	13.87		C
ANISOU	6952	CA	ALA	B	156	1728	1857	1685	94	-29	-28	C
ATOM	6954	CB	ALA	B	156	66.884	13.323	50.575	1.00	13.88		C
ANISOU	6954	CB	ALA	B	156	1673	1783	1815	19	-75	-91	C
ATOM	6977	C	ILE	B	157	66.494	9.432	54.217	1.00	13.23		C
ANISOU	6977	C	ILE	B	157	1685	1596	1744	13	146	-106	C
ATOM	6979	N	SER	B	158	66.814	10.480	54.970	1.00	12.13		N
ANISOU	6979	N	SER	B	158	1604	1384	1621	6	127	-37	N
ATOM	6981	CA	SER	B	158	66.092	10.699	56.225	1.00	12.23		C
ANISOU	6981	CA	SER	B	158	1542	1523	1580	30	37	18	C
ATOM	6983	CB	SER	B	158	66.655	9.823	57.342	1.00	12.86		C
ANISOU	6983	CB	SER	B	158	1640	1678	1568	27	39	-24	C
ATOM	6986	OG	SER	B	158	67.745	10.437	57.970	1.00	11.97		O
ANISOU	6986	OG	SER	B	158	1299	1403	1845	20	-59	181	O
ATOM	6988	C	SER	B	158	66.064	12.142	56.642	1.00	10.81		C
ANISOU	6988	C	SER	B	158	1329	1348	1428	52	18	55	C
ATOM	6989	O	SER	B	158	66.892	12.934	56.202	1.00	11.82		O
ANISOU	6989	O	SER	B	158	1345	1578	1567	251	122	56	O
ATOM	6990	N	LEU	B	159	65.088	12.475	57.481	1.00	9.46		N
ANISOU	6990	N	LEU	B	159	1213	1117	1261	-57	64	128	N
ATOM	6992	CA	LEU	B	159	64.879	13.787	58.029	1.00	9.04		C
ANISOU	6992	CA	LEU	B	159	1098	1189	1147	-26	16	82	C
ATOM	6994	CB	LEU	B	159	63.605	14.413	57.398	1.00	8.61		C
ANISOU	6994	CB	LEU	B	159	969	1151	1151	-97	79	188	C
ATOM	6997	CG	LEU	B	159	63.761	14.649	55.868	1.00	10.31		C
ANISOU	6997	CG	LEU	B	159	1332	1409	1174	-50	-118	25	C
ATOM	6999	CD1	LEU	B	159	62.421	15.004	55.226	1.00	12.39		C
ANISOU	6999	CD1	LEU	B	159	1511	1595	1602	-8	-35	227	C
ATOM	7003	CD2	LEU	B	159	64.708	15.846	55.696	1.00	13.41		C
ANISOU	7003	CD2	LEU	B	159	1552	1838	1705	-57	71	214	C
ATOM	7007	C	LEU	B	159	64.660	13.645	59.520	1.00	8.85		C
ANISOU	7007	C	LEU	B	159	1084	1147	1129	-8	-25	45	C
ATOM	7008	O	LEU	B	159	63.891	12.786	59.942	1.00	7.91		O
ANISOU	7008	O	LEU	B	159	1140	1062	803	-123	13	29	O
ATOM	7009	N	GLU	B	160	65.332	14.476	60.310	1.00	8.63		N
ANISOU	7009	N	GLU	B	160	1081	1059	1136	36	-25	69	N
ATOM	7011	CA	GLU	B	160	65.158	14.493	61.739	1.00	8.95		C
ANISOU	7011	CA	GLU	B	160	1115	1153	1130	72	-16	-32	C
ATOM	7013	CB	GLU	B	160	66.331	13.815	62.438	1.00	7.85		C
ANISOU	7013	CB	GLU	B	160	987	1021	973	64	71	39	C
ATOM	7016	CG	GLU	B	160	66.390	12.339	62.103	1.00	9.92		C
ANISOU	7016	CG	GLU	B	160	1125	1167	1477	-157	-37	38	C
ATOM	7019	CD	GLU	B	160	67.368	11.600	62.960	1.00	13.56		C
ANISOU	7019	CD	GLU	B	160	1471	1568	2110	-16	-165	141	C
ATOM	7020	OE1	GLU	B	160	68.420	12.139	63.361	1.00	11.79		O
ANISOU	7020	OE1	GLU	B	160	1364	1270	1843	114	25	-131	O
ATOM	7021	OE2	GLU	B	160	67.066	10.458	63.251	1.00	19.57		O
ANISOU	7021	OE2	GLU	B	160	2555	2049	2830	-104	-202	256	O
ATOM	7022	C	GLU	B	160	65.073	15.953	62.223	1.00	9.19		C
ANISOU	7022	C	GLU	B	160	1198	1123	1170	109	2	46	C
ATOM	7023	O	GLU	B	160	65.847	16.795	61.801	1.00	8.81		O
ANISOU	7023	O	GLU	B	160	1165	1090	1091	224	183	-91	O
ATOM	7024	N	GLU	B	161	64.105	16.230	63.101	1.00	7.95		N
ANISOU	7024	N	GLU	B	161	945	1136	939	63	6	108	N
ATOM	7026	CA	GLU	B	161	64.002	17.544	63.679	1.00	9.71		C
ANISOU	7026	CA	GLU	B	161	1269	1335	1083	73	-29	54	C
ATOM	7028	CB	GLU	B	161	62.541	17.931	63.962	1.00	10.03		C
ANISOU	7028	CB	GLU	B	161	1296	1308	1204	6	-27	34	C
ATOM	7031	CG	GLU	B	161	62.378	19.345	64.548	1.00	11.96		C
ANISOU	7031	CG	GLU	B	161	1668	1525	1351	68	109	21	C

ATOM	7034	CD	GLU B 161	62.621	20.471	63.580	1.00	10.40		C
ANISOU	7034	CD	GLU B 161	1366	1297	1288	77	-121	-23	C
ATOM	7035	OE1	GLU B 161	62.769	20.217	62.344	1.00	9.46		O
ANISOU	7035	OE1	GLU B 161	1144	1335	1113	315	-17	200	O
ATOM	7036	OE2	GLU B 161	62.698	21.630	64.081	1.00	11.19		O
ANISOU	7036	OE2	GLU B 161	1685	1516	1049	162	-158	-49	O
ATOM	7037	C	GLU B 161	64.831	17.672	64.977	1.00	9.61		C
ANISOU	7037	C	GLU B 161	1198	1288	1165	73	-60	48	C
ATOM	7038	O	GLU B 161	64.547	17.017	65.990	1.00	9.49		O
ANISOU	7038	O	GLU B 161	1036	1659	907	123	-157	48	O
ATOM	7039	N	LYS B 162	65.769	18.585	64.932	1.00	8.24		N
ANISOU	7039	N	LYS B 162	900	1202	1027	135	112	32	N
ATOM	7041	CA	LYS B 162	66.612	18.922	66.038	1.00	10.61		C
ANISOU	7041	CA	LYS B 162	1414	1348	1266	51	54	15	C
ATOM	7043	CB	LYS B 162	65.777	19.741	67.040	1.00	11.54		C
ANISOU	7043	CB	LYS B 162	1456	1471	1456	102	-6	36	C
ATOM	7046	CG	LYS B 162	65.558	21.165	66.523	1.00	15.09		C
ANISOU	7046	CG	LYS B 162	1991	1686	2055	126	-46	54	C
ATOM	7049	CD	LYS B 162	64.544	21.836	67.435	1.00	17.98		C
ANISOU	7049	CD	LYS B 162	2270	2386	2175	120	89	-28	C
ATOM	7052	CE	LYS B 162	63.865	23.039	66.780	1.00	19.21		C
ANISOU	7052	CE	LYS B 162	2468	2383	2447	120	47	101	C
ATOM	7055	NZ	LYS B 162	64.917	23.948	66.384	1.00	25.24		N
ANISOU	7055	NZ	LYS B 162	3210	2930	3447	-1	42	78	N
ATOM	7059	C	LYS B 162	67.227	17.716	66.718	1.00	11.03		C
ANISOU	7059	C	LYS B 162	1314	1513	1364	144	45	6	C
ATOM	7060	O	LYS B 162	67.126	17.581	67.951	1.00	11.36		O
ANISOU	7060	O	LYS B 162	1530	1578	1206	230	217	-21	O
ATOM	7061	N	PRO B 163	67.881	16.837	65.949	1.00	10.90		N
ANISOU	7061	N	PRO B 163	1369	1469	1300	5	62	-12	N
ATOM	7062	CA	PRO B 163	68.501	15.646	66.534	1.00	10.11		C
ANISOU	7062	CA	PRO B 163	1179	1379	1283	20	102	16	C
ATOM	7064	CB	PRO B 163	68.952	14.853	65.303	1.00	10.34		C
ANISOU	7064	CB	PRO B 163	1335	1295	1296	-121	-21	-45	C
ATOM	7067	CG	PRO B 163	69.193	15.867	64.337	1.00	11.48		C
ANISOU	7067	CG	PRO B 163	1511	1580	1269	9	-12	48	C
ATOM	7070	CD	PRO B 163	68.085	16.867	64.494	1.00	10.62		C
ANISOU	7070	CD	PRO B 163	1190	1536	1306	-21	149	22	C
ATOM	7073	C	PRO B 163	69.682	15.923	67.453	1.00	9.77		C
ANISOU	7073	C	PRO B 163	1237	1212	1262	-68	74	-20	C
ATOM	7074	O	PRO B 163	70.536	16.755	67.176	1.00	8.05		O
ANISOU	7074	O	PRO B 163	638	1151	1270	31	86	163	O
ATOM	7075	N	LEU B 164	69.704	15.244	68.586	1.00	9.04		N
ANISOU	7075	N	LEU B 164	1196	1040	1196	37	53	-2	N
ATOM	7077	CA	LEU B 164	70.811	15.393	69.491	1.00	11.39		C
ANISOU	7077	CA	LEU B 164	1511	1363	1453	7	34	-10	C
ATOM	7079	CB	LEU B 164	70.523	14.622	70.770	1.00	12.96		C
ANISOU	7079	CB	LEU B 164	1722	1676	1525	20	43	8	C
ATOM	7082	CG	LEU B 164	69.397	15.097	71.678	1.00	17.24		C
ANISOU	7082	CG	LEU B 164	2118	2230	2201	89	70	-32	C
ATOM	7084	CD1	LEU B 164	69.777	14.694	73.107	1.00	20.27		C
ANISOU	7084	CD1	LEU B 164	2686	2662	2351	-51	-52	-87	C
ATOM	7088	CD2	LEU B 164	69.152	16.549	71.571	1.00	20.80		C
ANISOU	7088	CD2	LEU B 164	2721	2523	2659	-3	125	-15	C
ATOM	7092	C	LEU B 164	72.106	14.910	68.853	1.00	10.34		C
ANISOU	7092	C	LEU B 164	1309	1312	1306	0	58	28	C
ATOM	7093	O	LEU B 164	73.202	15.461	69.140	1.00	11.48		O
ANISOU	7093	O	LEU B 164	1825	1369	1164	-68	-124	-274	O
ATOM	7094	N	GLU B 165	72.014	13.917	67.981	1.00	9.08		N
ANISOU	7094	N	GLU B 165	983	1208	1257	-135	7	-17	N
ATOM	7096	CA	GLU B 165	73.208	13.371	67.248	1.00	10.89		C

ANISOU	7096	CA	GLU B 165	1475	1357	1304	6	32	0	C
ATOM	7107	C	GLU B 165	72.803	13.407	65.771	1.00	10.15		C
ANISOU	7107	C	GLU B 165	1363	1274	1219	-38	11	-4	C
ATOM	7108	O	GLU B 165	72.297	12.454	65.194	1.00	9.49		O
ANISOU	7108	O	GLU B 165	1186	1135	1282	-92	64	18	O
ATOM	7109	N	PRO B 166	73.017	14.558	65.180	1.00	9.27		N
ANISOU	7109	N	PRO B 166	1240	1180	1101	-12	34	2	N
ATOM	7110	CA	PRO B 166	72.707	14.753	63.767	1.00	8.50		C
ANISOU	7110	CA	PRO B 166	1016	1168	1045	6	-19	35	C
ATOM	7112	CB	PRO B 166	73.184	16.161	63.479	1.00	8.60		C
ANISOU	7112	CB	PRO B 166	1047	1184	1034	-39	6	-54	C
ATOM	7115	CG	PRO B 166	73.454	16.820	64.802	1.00	10.24		C
ANISOU	7115	CG	PRO B 166	1479	1335	1076	-97	23	16	C
ATOM	7118	CD	PRO B 166	73.566	15.741	65.851	1.00	9.86		C
ANISOU	7118	CD	PRO B 166	1331	1166	1248	-10	-66	38	C
ATOM	7121	C	PRO B 166	73.433	13.769	62.861	1.00	8.82		C
ANISOU	7121	C	PRO B 166	1090	1200	1058	-9	7	57	C
ATOM	7122	O	PRO B 166	74.650	13.478	63.053	1.00	9.73		O
ANISOU	7122	O	PRO B 166	1035	1533	1128	148	169	21	O
ATOM	7123	N	LYS B 167	72.711	13.280	61.860	1.00	8.94		N
ANISOU	7123	N	LYS B 167	1119	1142	1135	-82	210	54	N
ATOM	7125	CA	LYS B 167	73.279	12.330	60.928	1.00	9.63		C
ANISOU	7125	CA	LYS B 167	1278	1123	1258	39	90	-27	C
ATOM	7127	CB	LYS B 167	72.183	11.470	60.289	1.00	8.15		C
ANISOU	7127	CB	LYS B 167	960	1010	1126	111	128	-110	C
ATOM	7130	CG	LYS B 167	71.617	10.439	61.327	1.00	11.24		C
ANISOU	7130	CG	LYS B 167	1544	1370	1354	94	112	-31	C
ATOM	7133	CD	LYS B 167	70.366	9.721	60.827	1.00	13.95		C
ANISOU	7133	CD	LYS B 167	1691	1784	1825	-4	49	-54	C
ATOM	7143	C	LYS B 167	74.144	12.979	59.848	1.00	8.82		C
ANISOU	7143	C	LYS B 167	1025	1081	1244	-1	88	-20	C
ATOM	7144	O	LYS B 167	74.781	12.256	59.092	1.00	10.84		O
ANISOU	7144	O	LYS B 167	1677	1095	1344	24	131	-56	O
ATOM	7145	N	SER B 168	74.090	14.317	59.728	1.00	7.84		N
ANISOU	7145	N	SER B 168	858	1062	1056	-27	-62	32	N
ATOM	7147	CA	SER B 168	74.913	15.048	58.788	1.00	8.49		C
ANISOU	7147	CA	SER B 168	964	1151	1110	2	-31	-32	C
ATOM	7149	CB	SER B 168	74.321	15.086	57.392	1.00	7.62		C
ANISOU	7149	CB	SER B 168	888	1013	992	-25	-44	-109	C
ATOM	7152	OG	SER B 168	73.281	16.077	57.307	1.00	8.98		O
ANISOU	7152	OG	SER B 168	826	1444	1140	53	-406	-271	O
ATOM	7154	C	SER B 168	75.000	16.498	59.258	1.00	8.20		C
ANISOU	7154	C	SER B 168	925	1116	1075	27	-72	-66	C
ATOM	7155	O	SER B 168	74.394	16.864	60.255	1.00	9.84		O
ANISOU	7155	O	SER B 168	1046	1365	1325	-134	2	-118	O
ATOM	7156	N	ASN B 169	75.720	17.311	58.516	1.00	8.34		N
ANISOU	7156	N	ASN B 169	1082	1134	953	33	-28	12	N
ATOM	7158	CA	ASN B 169	75.830	18.723	58.792	1.00	9.44		C
ANISOU	7158	CA	ASN B 169	1280	1219	1087	60	21	-29	C
ATOM	7160	CB	ASN B 169	77.288	19.190	58.675	1.00	10.02		C
ANISOU	7160	CB	ASN B 169	1439	1222	1145	1	-50	-65	C
ATOM	7163	CG	ASN B 169	78.135	18.686	59.862	1.00	11.94		C
ANISOU	7163	CG	ASN B 169	1572	1549	1415	80	-166	-103	C
ATOM	7164	OD1	ASN B 169	77.697	18.777	61.022	1.00	16.26		O
ANISOU	7164	OD1	ASN B 169	2408	2285	1485	95	-122	102	O
ATOM	7165	ND2	ASN B 169	79.280	18.144	59.581	1.00	10.28		N
ANISOU	7165	ND2	ASN B 169	1387	1439	1079	3	-271	-63	N
ATOM	7168	C	ASN B 169	74.902	19.558	57.911	1.00	9.68		C
ANISOU	7168	C	ASN B 169	1384	1215	1077	-22	-80	-15	C
ATOM	7169	O	ASN B 169	75.076	20.779	57.793	1.00	10.98		O
ANISOU	7169	O	ASN B 169	1808	1180	1180	-171	-94	-73	O

ATOM	7170	N	TYR B 170	73.947	18.924	57.249	1.00	8.76		N
ANISOU	7170	N	TYR B 170	1193	1035	1100	-16	82	-62	N
ATOM	7172	CA	TYR B 170	73.041	19.648	56.357	1.00	6.97		C
ANISOU	7172	CA	TYR B 170	859	947	839	-65	20	-13	C
ATOM	7174	CB	TYR B 170	72.838	18.873	55.047	1.00	7.14		C
ANISOU	7174	CB	TYR B 170	744	1100	869	27	64	-56	C
ATOM	7177	CG	TYR B 170	74.049	19.087	54.169	1.00	6.20		C
ANISOU	7177	CG	TYR B 170	682	865	806	-82	28	84	C
ATOM	7178	CD1	TYR B 170	75.125	18.210	54.227	1.00	7.09		C
ANISOU	7178	CD1	TYR B 170	881	1015	797	-42	-24	-21	C
ATOM	7180	CE1	TYR B 170	76.267	18.445	53.502	1.00	6.23		C
ANISOU	7180	CE1	TYR B 170	789	825	751	-21	92	-81	C
ATOM	7182	CZ	TYR B 170	76.319	19.611	52.703	1.00	8.76		C
ANISOU	7182	CZ	TYR B 170	1264	1229	833	-31	-143	-45	C
ATOM	7185	CE2	TYR B 170	75.288	20.489	52.678	1.00	8.94		C
ANISOU	7185	CE2	TYR B 170	1111	1124	1159	-72	148	-78	C
ATOM	7187	CD2	TYR B 170	74.161	20.230	53.421	1.00	7.63		C
ANISOU	7187	CD2	TYR B 170	1007	924	965	-99	42	-17	C
ATOM	7189	C	TYR B 170	71.705	19.966	56.998	1.00	8.15		C
ANISOU	7189	C	TYR B 170	980	1052	1062	-14	4	-7	C
ATOM	7190	O	TYR B 170	70.939	19.041	57.332	1.00	9.22		O
ANISOU	7190	O	TYR B 170	1159	1096	1248	-254	192	159	O
ATOM	7191	N	ALA B 171	71.437	21.251	57.213	1.00	7.85		N
ANISOU	7191	N	ALA B 171	922	915	1145	-85	-3	128	N
ATOM	7193	CA	ALA B 171	70.157	21.703	57.779	1.00	6.04		C
ANISOU	7193	CA	ALA B 171	830	722	741	-16	-7	129	C
ATOM	7195	CB	ALA B 171	70.345	23.032	58.562	1.00	7.20		C
ANISOU	7195	CB	ALA B 171	910	977	845	34	-101	113	C
ATOM	7199	C	ALA B 171	69.182	21.939	56.641	1.00	7.69		C
ANISOU	7199	C	ALA B 171	914	1065	940	-10	-11	60	C
ATOM	7200	O	ALA B 171	69.585	22.371	55.569	1.00	9.49		O
ANISOU	7200	O	ALA B 171	1245	1401	958	41	-59	75	O
ATOM	7201	N	VAL B 172	67.904	21.754	56.929	1.00	7.02		N
ANISOU	7201	N	VAL B 172	877	941	849	-86	37	83	N
ATOM	7203	CA	VAL B 172	66.820	22.038	55.994	1.00	7.98		C
ANISOU	7203	CA	VAL B 172	986	1067	978	-7	60	93	C
ATOM	7205	CB	VAL B 172	65.689	21.006	56.048	1.00	7.69		C
ANISOU	7205	CB	VAL B 172	860	985	1074	13	10	81	C
ATOM	7207	CG1	VAL B 172	64.547	21.391	55.088	1.00	7.84		C
ANISOU	7207	CG1	VAL B 172	1162	1028	787	-190	-64	125	C
ATOM	7211	CG2	VAL B 172	66.192	19.558	55.778	1.00	8.46		C
ANISOU	7211	CG2	VAL B 172	1103	1224	887	-156	204	-81	C
ATOM	7215	C	VAL B 172	66.365	23.443	56.381	1.00	8.06		C
ANISOU	7215	C	VAL B 172	967	1038	1058	-44	8	38	C
ATOM	7216	O	VAL B 172	65.849	23.672	57.484	1.00	7.37		O
ANISOU	7216	O	VAL B 172	858	896	1044	0	-160	147	O
ATOM	7217	N	THR B 173	66.585	24.394	55.469	1.00	9.20		N
ANISOU	7217	N	THR B 173	1211	1258	1024	32	28	12	N
ATOM	7219	CA	THR B 173	66.371	25.812	55.744	1.00	9.64		C
ANISOU	7219	CA	THR B 173	1185	1226	1249	26	17	75	C
ATOM	7221	CB	THR B 173	67.023	26.735	54.707	1.00	9.14		C
ANISOU	7221	CB	THR B 173	1041	1285	1147	96	122	-4	C
ATOM	7223	OG1	THR B 173	66.266	26.732	53.499	1.00	10.36		O
ANISOU	7223	OG1	THR B 173	1012	1431	1493	-10	304	28	O
ATOM	7225	CG2	THR B 173	68.470	26.306	54.352	1.00	10.18		C
ANISOU	7225	CG2	THR B 173	1304	1372	1190	-76	229	162	C
ATOM	7229	C	THR B 173	64.866	26.124	55.842	1.00	8.67		C
ANISOU	7229	C	THR B 173	1013	1152	1126	44	72	68	C
ATOM	7230	O	THR B 173	64.072	25.302	55.440	1.00	9.73		O
ANISOU	7230	O	THR B 173	1318	1015	1363	113	-24	71	O
ATOM	7231	N	GLY B 174	64.521	27.335	56.293	1.00	9.12		N

ANISOU	7231	N	GLY	B	174	1083	1193	1187	-43	-31	16	N
ATOM	7233	CA	GLY	B	174	63.118	27.788	56.507	1.00	8.23		C
ANISOU	7233	CA	GLY	B	174	998	908	1220	-40	-25	-18	C
ATOM	7236	C	GLY	B	174	62.455	28.303	55.233	1.00	8.36		C
ANISOU	7236	C	GLY	B	174	950	962	1263	-58	-50	-3	C
ATOM	7237	O	GLY	B	174	61.864	29.391	55.196	1.00	9.09		O
ANISOU	7237	O	GLY	B	174	902	1011	1540	-22	-184	-212	O
ATOM	7238	N	LEU	B	175	62.550	27.547	54.168	1.00	8.58		N
ANISOU	7238	N	LEU	B	175	1052	932	1275	102	-60	-34	N
ATOM	7240	CA	LEU	B	175	61.951	27.902	52.868	1.00	9.59		C
ANISOU	7240	CA	LEU	B	175	1235	1096	1313	37	33	-36	C
ATOM	7242	CB	LEU	B	175	62.951	28.584	51.975	1.00	9.42		C
ANISOU	7242	CB	LEU	B	175	1080	1117	1381	-85	-51	-70	C
ATOM	7245	CG	LEU	B	175	62.330	28.947	50.646	1.00	11.58		C
ANISOU	7245	CG	LEU	B	175	1567	1326	1505	60	111	-63	C
ATOM	7247	CD1	LEU	B	175	61.151	29.961	50.721	1.00	8.89		C
ANISOU	7247	CD1	LEU	B	175	759	1276	1341	-262	58	54	C
ATOM	7251	CD2	LEU	B	175	63.498	29.481	49.870	1.00	12.70		C
ANISOU	7251	CD2	LEU	B	175	1717	1586	1521	-282	120	-139	C
ATOM	7255	C	LEU	B	175	61.462	26.629	52.196	1.00	8.98		C
ANISOU	7255	C	LEU	B	175	1141	1076	1194	10	33	-71	C
ATOM	7256	O	LEU	B	175	62.238	25.714	52.008	1.00	10.88		O
ANISOU	7256	O	LEU	B	175	1319	1383	1430	24	167	-204	O
ATOM	7257	N	TYR	B	176	60.183	26.555	51.939	1.00	7.28		N
ANISOU	7257	N	TYR	B	176	905	773	1086	106	46	-100	N
ATOM	7259	CA	TYR	B	176	59.497	25.326	51.518	1.00	8.16		C
ANISOU	7259	CA	TYR	B	176	916	997	1185	37	102	-9	C
ATOM	7261	CB	TYR	B	176	58.786	24.724	52.739	1.00	7.87		C
ANISOU	7261	CB	TYR	B	176	937	899	1154	-8	-36	100	C
ATOM	7264	CG	TYR	B	176	59.526	24.715	54.008	1.00	7.97		C
ANISOU	7264	CG	TYR	B	176	991	841	1196	-64	-12	-29	C
ATOM	7265	CD1	TYR	B	176	59.388	25.734	54.907	1.00	9.89		C
ANISOU	7265	CD1	TYR	B	176	1240	1304	1213	268	120	2	C
ATOM	7267	CE1	TYR	B	176	60.079	25.737	56.091	1.00	8.98		C
ANISOU	7267	CE1	TYR	B	176	815	1243	1353	35	-113	-69	C
ATOM	7269	CZ	TYR	B	176	60.968	24.694	56.398	1.00	8.89		C
ANISOU	7269	CZ	TYR	B	176	988	1207	1182	69	32	27	C
ATOM	7270	OH	TYR	B	176	61.655	24.705	57.632	1.00	7.40		O
ANISOU	7270	OH	TYR	B	176	372	1252	1185	-104	32	178	O
ATOM	7272	CE2	TYR	B	176	61.147	23.683	55.518	1.00	7.38		C
ANISOU	7272	CE2	TYR	B	176	451	1022	1331	-294	-21	-15	C
ATOM	7274	CD2	TYR	B	176	60.485	23.705	54.295	1.00	8.70		C
ANISOU	7274	CD2	TYR	B	176	1083	1052	1167	9	-55	139	C
ATOM	7276	C	TYR	B	176	58.472	25.580	50.419	1.00	7.85		C
ANISOU	7276	C	TYR	B	176	1068	896	1017	-52	111	23	C
ATOM	7277	O	TYR	B	176	57.621	26.490	50.539	1.00	8.80		O
ANISOU	7277	O	TYR	B	176	1127	1079	1138	34	154	26	O
ATOM	7278	N	PHE	B	177	58.536	24.797	49.335	1.00	7.19		N
ANISOU	7278	N	PHE	B	177	1047	787	896	-43	75	2	N
ATOM	7280	CA	PHE	B	177	57.627	24.921	48.216	1.00	7.33		C
ANISOU	7280	CA	PHE	B	177	818	932	1032	3	46	-7	C
ATOM	7282	CB	PHE	B	177	58.419	25.078	46.915	1.00	7.10		C
ANISOU	7282	CB	PHE	B	177	974	939	781	-67	-115	62	C
ATOM	7285	CG	PHE	B	177	59.066	26.422	46.767	1.00	7.98		C
ANISOU	7285	CG	PHE	B	177	959	973	1100	-118	-151	-43	C
ATOM	7286	CD1	PHE	B	177	60.281	26.688	47.384	1.00	8.17		C
ANISOU	7286	CD1	PHE	B	177	724	1045	1335	12	-101	-84	C
ATOM	7288	CE1	PHE	B	177	60.852	27.910	47.240	1.00	9.74		C
ANISOU	7288	CE1	PHE	B	177	896	1193	1610	-64	-197	-26	C
ATOM	7290	CZ	PHE	B	177	60.242	28.929	46.525	1.00	10.02		C
ANISOU	7290	CZ	PHE	B	177	1083	1433	1288	-135	-83	144	C

ATOM	7296	C	PHE B 177	56.769	23.644	48.140	1.00	7.12		C
ANISOU	7296	C	PHE B 177	967	821	915	39	12	-138	C
ATOM	7297	O	PHE B 177	57.318	22.531	48.200	1.00	8.86		O
ANISOU	7297	O	PHE B 177	1163	1024	1177	162	-173	-113	O
ATOM	7298	N	TYR B 178	55.438	23.808	48.103	1.00	5.89		N
ANISOU	7298	N	TYR B 178	673	838	726	40	-204	-154	N
ATOM	7302	CB	TYR B 178	53.773	22.537	49.407	1.00	8.00		C
ANISOU	7302	CB	TYR B 178	1075	946	1017	91	45	-20	C
ATOM	7305	CG	TYR B 178	54.683	22.338	50.579	1.00	6.73		C
ANISOU	7305	CG	TYR B 178	590	1082	885	-94	167	42	C
ATOM	7306	CD1	TYR B 178	54.890	23.343	51.492	1.00	8.96		C
ANISOU	7306	CD1	TYR B 178	842	1200	1362	161	26	33	C
ATOM	7308	CE1	TYR B 178	55.685	23.176	52.554	1.00	7.92		C
ANISOU	7308	CE1	TYR B 178	1075	1280	653	45	174	-51	C
ATOM	7310	CZ	TYR B 178	56.347	21.956	52.733	1.00	9.90		C
ANISOU	7310	CZ	TYR B 178	1269	1275	1216	-62	47	-48	C
ATOM	7311	OH	TYR B 178	57.152	21.787	53.814	1.00	11.41		O
ANISOU	7311	OH	TYR B 178	1388	1768	1175	241	-23	8	O
ATOM	7313	CE2	TYR B 178	56.175	20.933	51.836	1.00	10.09		C
ANISOU	7313	CE2	TYR B 178	1238	1289	1305	-31	-3	-55	C
ATOM	7315	CD2	TYR B 178	55.317	21.143	50.756	1.00	7.48		C
ANISOU	7315	CD2	TYR B 178	803	969	1067	-285	218	96	C
ATOM	7375	CG2	VAL B 182	51.971	21.111	52.994	1.00	8.00		C
ANISOU	7375	CG2	VAL B 182	546	1403	1087	-54	-64	83	C
ATOM	7422	CG2	ILE B 185	51.599	16.073	55.179	1.00	12.67		C
ANISOU	7422	CG2	ILE B 185	1651	1554	1609	110	-11	-97	C
ATOM	7428	N	ALA B 186	49.151	18.085	56.330	1.00	10.77		N
ANISOU	7428	N	ALA B 186	1360	1340	1389	4	-98	-48	N
ATOM	7430	CA	ALA B 186	49.169	18.840	57.574	1.00	11.68		C
ANISOU	7430	CA	ALA B 186	1479	1473	1484	8	-31	-4	C
ATOM	7432	CB	ALA B 186	49.225	20.346	57.254	1.00	11.61		C
ANISOU	7432	CB	ALA B 186	1626	1449	1335	45	6	-194	C
ATOM	7436	C	ALA B 186	47.988	18.476	58.461	1.00	12.71		C
ANISOU	7436	C	ALA B 186	1674	1579	1575	28	16	-47	C
ATOM	7437	O	ALA B 186	48.149	18.327	59.678	1.00	12.14		O
ANISOU	7437	O	ALA B 186	1516	1560	1538	-30	-15	-18	O
ATOM	7438	N	ARG B 187	46.842	18.242	57.825	1.00	13.18		N
ANISOU	7438	N	ARG B 187	1625	1686	1695	-19	-23	16	N
ATOM	7474	N	LEU B 189	48.515	15.399	60.551	1.00	16.10		N
ANISOU	7474	N	LEU B 189	2063	2029	2025	-81	98	63	N
ATOM	7476	CA	LEU B 189	49.577	15.457	61.549	1.00	16.49		C
ANISOU	7476	CA	LEU B 189	2101	2072	2091	-53	6	33	C
ATOM	7478	CB	LEU B 189	50.490	16.644	61.274	1.00	16.83		C
ANISOU	7478	CB	LEU B 189	2170	2105	2117	-22	8	79	C
ATOM	7481	CG	LEU B 189	51.338	16.526	60.036	1.00	18.75		C
ANISOU	7481	CG	LEU B 189	2537	2344	2243	22	34	41	C
ATOM	7483	CD1	LEU B 189	52.315	17.642	60.087	1.00	20.29		C
ANISOU	7483	CD1	LEU B 189	2490	2703	2517	-87	-45	39	C
ATOM	7487	CD2	LEU B 189	52.052	15.217	59.871	1.00	19.13		C
ANISOU	7487	CD2	LEU B 189	2221	2547	2498	103	0	85	C
ATOM	7491	C	LEU B 189	49.075	15.546	63.004	1.00	16.86		C
ANISOU	7491	C	LEU B 189	2192	2091	2122	-52	27	-25	C
ATOM	7492	O	LEU B 189	47.990	16.075	63.292	1.00	16.15		O
ANISOU	7492	O	LEU B 189	2169	2171	1795	-229	210	30	O
ATOM	7493	N	LYS B 190	49.883	14.966	63.876	1.00	17.97		N
ANISOU	7493	N	LYS B 190	2412	2211	2202	-56	-47	-57	N
ATOM	7495	CA	LYS B 190	49.706	15.010	65.308	1.00	19.53		C
ANISOU	7495	CA	LYS B 190	2539	2433	2448	-42	48	19	C
ATOM	7513	C	LYS B 190	50.967	15.681	65.884	1.00	19.71		C
ANISOU	7513	C	LYS B 190	2529	2527	2433	10	-18	39	C
ATOM	7514	O	LYS B 190	52.050	15.627	65.306	1.00	18.46		O

ANISOU	7514	O	LYS	B	190	2348	2216	2447	46	-19	6	O
ATOM	7515	N	PRO	B	191	50.837	16.297	67.037	1.00	20.60		N
ANISOU	7515	N	PRO	B	191	2647	2543	2636	18	4	-38	N
ATOM	7516	CA	PRO	B	191	51.992	16.922	67.667	1.00	20.66		C
ANISOU	7516	CA	PRO	B	191	2546	2636	2665	-25	31	-13	C
ATOM	7518	CB	PRO	B	191	51.443	17.431	68.993	1.00	21.14		C
ANISOU	7518	CB	PRO	B	191	2673	2788	2568	-27	-13	43	C
ATOM	7521	CG	PRO	B	191	49.990	17.490	68.831	1.00	20.59		C
ANISOU	7521	CG	PRO	B	191	2543	2680	2597	0	31	8	C
ATOM	7524	CD	PRO	B	191	49.629	16.407	67.876	1.00	20.66		C
ANISOU	7524	CD	PRO	B	191	2619	2631	2598	-21	44	14	C
ATOM	7527	C	PRO	B	191	53.109	15.954	67.936	1.00	20.82		C
ANISOU	7527	C	PRO	B	191	2686	2586	2636	-36	8	43	C
ATOM	7528	O	PRO	B	191	52.888	14.802	68.281	1.00	20.54		O
ANISOU	7528	O	PRO	B	191	2721	2529	2551	-233	97	63	O
ATOM	7529	N	SER	B	192	54.334	16.452	67.791	1.00	20.18		N
ANISOU	7529	N	SER	B	192	2515	2559	2592	-49	4	32	N
ATOM	7531	CA	SER	B	192	55.522	15.645	68.009	1.00	20.49		C
ANISOU	7531	CA	SER	B	192	2640	2562	2581	-12	-12	41	C
ATOM	7533	CB	SER	B	192	56.676	16.336	67.312	1.00	20.07		C
ANISOU	7533	CB	SER	B	192	2586	2530	2508	35	-27	-21	C
ATOM	7536	OG	SER	B	192	56.924	17.600	67.915	1.00	16.60		O
ANISOU	7536	OG	SER	B	192	2175	1953	2177	12	-75	238	O
ATOM	7538	C	SER	B	192	55.853	15.576	69.503	1.00	22.31		C
ANISOU	7538	C	SER	B	192	2911	2820	2745	11	10	20	C
ATOM	7539	O	SER	B	192	55.197	16.183	70.328	1.00	22.56		O
ANISOU	7539	O	SER	B	192	3054	2894	2621	-49	120	130	O
ATOM	7540	N	PRO	B	193	56.902	14.864	69.845	1.00	23.94		N
ANISOU	7540	N	PRO	B	193	3070	3054	2971	40	-40	16	N
ATOM	7541	CA	PRO	B	193	57.349	14.879	71.229	1.00	25.06		C
ANISOU	7541	CA	PRO	B	193	3188	3203	3128	20	-21	-8	C
ATOM	7543	CB	PRO	B	193	58.548	13.935	71.219	1.00	25.63		C
ANISOU	7543	CB	PRO	B	193	3310	3260	3164	53	-43	-6	C
ATOM	7546	CG	PRO	B	193	58.433	13.132	69.969	1.00	25.15		C
ANISOU	7546	CG	PRO	B	193	3262	3149	3144	15	-75	35	C
ATOM	7549	CD	PRO	B	193	57.732	14.009	68.980	1.00	24.02		C
ANISOU	7549	CD	PRO	B	193	3047	3038	3040	20	-32	49	C
ATOM	7552	C	PRO	B	193	57.709	16.352	71.624	1.00	25.81		C
ANISOU	7552	C	PRO	B	193	3309	3289	3207	19	7	2	C
ATOM	7553	O	PRO	B	193	57.427	16.755	72.732	1.00	27.82		O
ANISOU	7553	O	PRO	B	193	3603	3576	3388	100	-107	-123	O
ATOM	7554	N	ARG	B	194	58.272	17.162	70.734	1.00	25.10		N
ANISOU	7554	N	ARG	B	194	3178	3155	3204	9	-29	-2	N
ATOM	7556	CA	ARG	B	194	58.520	18.563	71.066	1.00	24.00		C
ANISOU	7556	CA	ARG	B	194	3013	3039	3065	47	-20	-6	C
ATOM	7558	CB	ARG	B	194	59.263	19.245	69.910	1.00	23.37		C
ANISOU	7558	CB	ARG	B	194	3000	2954	2923	22	-39	-13	C
ATOM	7561	CG	ARG	B	194	60.797	19.042	69.907	1.00	24.76		C
ANISOU	7561	CG	ARG	B	194	3153	3109	3144	-7	32	-2	C
ATOM	7564	CD	ARG	B	194	61.541	19.205	68.503	1.00	28.11		C
ANISOU	7564	CD	ARG	B	194	3686	3508	3487	44	98	88	C
ATOM	7567	NE	ARG	B	194	62.228	17.946	68.264	1.00	28.35		N
ANISOU	7567	NE	ARG	B	194	3706	3686	3377	-25	76	-27	N
ATOM	7569	CZ	ARG	B	194	61.689	16.907	67.652	1.00	25.85		C
ANISOU	7569	CZ	ARG	B	194	3267	3480	3074	-14	44	-16	C
ATOM	7570	NH1	ARG	B	194	60.494	16.982	67.031	1.00	22.00		N
ANISOU	7570	NH1	ARG	B	194	2562	3096	2700	39	326	308	N
ATOM	7573	NH2	ARG	B	194	62.389	15.804	67.601	1.00	27.37		N
ANISOU	7573	NH2	ARG	B	194	3325	3587	3486	89	-120	73	N
ATOM	7576	C	ARG	B	194	57.203	19.345	71.396	1.00	22.88		C
ANISOU	7576	C	ARG	B	194	2907	2897	2887	7	-6	-14	C

ATOM	7577	O	ARG B 194	57.234	20.435	71.913	1.00	23.57		O
ANISOU	7577	O	ARG B 194	3005	2976	2974	54	26	-34	O
ATOM	7578	N	GLY B 195	56.058	18.788	71.086	1.00	20.97		N
ANISOU	7578	N	GLY B 195	2695	2630	2642	73	17	64	N
ATOM	7580	CA	GLY B 195	54.792	19.484	71.270	1.00	20.22		C
ANISOU	7580	CA	GLY B 195	2630	2569	2484	36	105	46	C
ATOM	7583	C	GLY B 195	54.392	20.377	70.099	1.00	18.88		C
ANISOU	7583	C	GLY B 195	2422	2417	2332	138	59	-8	C
ATOM	7584	O	GLY B 195	53.606	21.319	70.264	1.00	20.12		O
ANISOU	7584	O	GLY B 195	2613	2666	2364	157	246	-57	O
ATOM	7585	N	GLU B 196	54.940	20.122	68.914	1.00	16.10		N
ANISOU	7585	N	GLU B 196	2099	2042	1973	118	52	42	N
ATOM	7587	CA	GLU B 196	54.616	20.910	67.741	1.00	14.77		C
ANISOU	7587	CA	GLU B 196	1898	1860	1852	52	35	-23	C
ATOM	7589	CB	GLU B 196	55.843	21.648	67.191	1.00	14.83		C
ANISOU	7589	CB	GLU B 196	1880	1821	1934	56	45	4	C
ATOM	7592	CG	GLU B 196	56.669	22.388	68.189	1.00	19.90		C
ANISOU	7592	CG	GLU B 196	2487	2571	2499	24	-103	77	C
ATOM	7595	CD	GLU B 196	56.042	23.677	68.595	1.00	25.07		C
ANISOU	7595	CD	GLU B 196	3348	2966	3209	119	21	-124	C
ATOM	7596	OE1	GLU B 196	55.371	24.369	67.759	1.00	25.27		O
ANISOU	7596	OE1	GLU B 196	3342	2931	3326	147	64	59	O
ATOM	7597	OE2	GLU B 196	56.216	23.981	69.772	1.00	31.30		O
ANISOU	7597	OE2	GLU B 196	4387	3910	3594	39	-188	43	O
ATOM	7598	C	GLU B 196	54.162	20.063	66.576	1.00	12.42		C
ANISOU	7598	C	GLU B 196	1683	1560	1473	-3	71	39	C
ATOM	7599	O	GLU B 196	54.545	18.886	66.439	1.00	13.86		O
ANISOU	7599	O	GLU B 196	2002	1857	1407	240	15	111	O
ATOM	7600	N	LEU B 197	53.391	20.702	65.726	1.00	9.67		N
ANISOU	7600	N	LEU B 197	1144	1146	1384	34	104	4	N
ATOM	7602	CA	LEU B 197	53.060	20.208	64.403	1.00	10.48		C
ANISOU	7602	CA	LEU B 197	1328	1283	1369	63	16	40	C
ATOM	7604	CB	LEU B 197	51.748	20.792	63.940	1.00	11.54		C
ANISOU	7604	CB	LEU B 197	1395	1455	1533	61	74	157	C
ATOM	7607	CG	LEU B 197	50.648	20.478	64.942	1.00	16.47		C
ANISOU	7607	CG	LEU B 197	2208	2160	1890	58	123	-15	C
ATOM	7609	CD1	LEU B 197	49.393	21.367	64.753	1.00	19.37		C
ANISOU	7609	CD1	LEU B 197	2276	2531	2549	68	-62	-62	C
ATOM	7613	CD2	LEU B 197	50.295	18.970	64.876	1.00	17.62		C
ANISOU	7613	CD2	LEU B 197	2385	2132	2175	-149	187	94	C
ATOM	7617	C	LEU B 197	54.192	20.610	63.465	1.00	9.52		C
ANISOU	7617	C	LEU B 197	1237	1222	1156	131	25	75	C
ATOM	7618	O	LEU B 197	54.329	21.789	63.089	1.00	8.44		O
ANISOU	7618	O	LEU B 197	969	1215	1022	118	165	10	O
ATOM	7619	N	GLU B 198	55.050	19.628	63.166	1.00	10.81		N
ANISOU	7619	N	GLU B 198	1525	1299	1283	96	112	112	N
ATOM	7621	CA	GLU B 198	56.340	19.832	62.524	1.00	10.00		C
ANISOU	7621	CA	GLU B 198	1220	1247	1332	90	-30	-9	C
ATOM	7623	CB	GLU B 198	57.316	18.708	62.964	1.00	11.34		C
ANISOU	7623	CB	GLU B 198	1377	1460	1470	87	60	37	C
ATOM	7626	CG	GLU B 198	57.437	18.462	64.458	1.00	12.25		C
ANISOU	7626	CG	GLU B 198	1430	1534	1688	199	-126	37	C
ATOM	7629	CD	GLU B 198	58.392	19.393	65.172	1.00	15.83		C
ANISOU	7629	CD	GLU B 198	1906	1996	2110	55	-95	26	C
ATOM	7630	OE1	GLU B 198	58.756	20.454	64.601	1.00	15.70		O
ANISOU	7630	OE1	GLU B 198	1945	2094	1925	70	119	269	O
ATOM	7631	OE2	GLU B 198	58.728	19.057	66.351	1.00	15.42		O
ANISOU	7631	OE2	GLU B 198	1714	2197	1949	434	-74	85	O
ATOM	7632	C	GLU B 198	56.364	19.910	60.996	1.00	8.74		C
ANISOU	7632	C	GLU B 198	1028	1124	1168	89	13	94	C
ATOM	7633	O	GLU B 198	55.772	19.043	60.264	1.00	8.91		O

ANISOU	7633	O	GLU B 198	880	1247	1255	144	44	82	O
ATOM	7634	N	ILE B 199	57.142	20.865	60.491	1.00	8.42		N
ANISOU	7634	N	ILE B 199	1074	1019	1106	29	-219	0	N
ATOM	7636	CA	ILE B 199	57.311	20.958	59.030	1.00	8.38		C
ANISOU	7636	CA	ILE B 199	1055	1031	1097	-48	54	47	C
ATOM	7638	CB	ILE B 199	58.004	22.290	58.569	1.00	8.06		C
ANISOU	7638	CB	ILE B 199	1021	947	1091	80	-59	34	C
ATOM	7640	CG1	ILE B 199	57.705	22.548	57.084	1.00	7.42		C
ANISOU	7640	CG1	ILE B 199	895	992	931	-143	35	31	C
ATOM	7643	CD1	ILE B 199	56.264	22.818	56.845	1.00	9.09		C
ANISOU	7643	CD1	ILE B 199	1284	1148	1019	233	-24	44	C
ATOM	7647	CG2	ILE B 199	59.536	22.259	58.748	1.00	9.61		C
ANISOU	7647	CG2	ILE B 199	1023	1095	1531	-125	-15	53	C
ATOM	7651	C	ILE B 199	58.105	19.735	58.593	1.00	8.98		C
ANISOU	7651	C	ILE B 199	1194	1130	1087	25	-70	26	C
ATOM	7652	O	ILE B 199	57.955	19.231	57.520	1.00	9.05		O
ANISOU	7652	O	ILE B 199	1443	1006	989	103	-139	85	O
ATOM	7653	N	THR B 200	58.956	19.233	59.468	1.00	9.37		N
ANISOU	7653	N	THR B 200	1308	1232	1017	123	-82	13	N
ATOM	7655	CA	THR B 200	59.813	18.165	59.104	1.00	10.32		C
ANISOU	7655	CA	THR B 200	1351	1404	1164	38	-16	35	C
ATOM	7657	CB	THR B 200	60.865	18.013	60.206	1.00	9.50		C
ANISOU	7657	CB	THR B 200	1192	1346	1071	108	-103	-54	C
ATOM	7659	OG1	THR B 200	61.743	19.168	60.167	1.00	10.06		O
ANISOU	7659	OG1	THR B 200	1261	1636	926	279	-26	-46	O
ATOM	7661	CG2	THR B 200	61.774	16.795	60.006	1.00	13.50		C
ANISOU	7661	CG2	THR B 200	1722	1822	1584	108	-69	-158	C
ATOM	7665	C	THR B 200	58.946	16.926	58.876	1.00	9.17		C
ANISOU	7665	C	THR B 200	1248	1188	1045	21	35	92	C
ATOM	7666	O	THR B 200	59.226	16.135	58.012	1.00	9.46		O
ANISOU	7666	O	THR B 200	1201	1233	1158	71	204	311	O
ATOM	7667	N	ASP B 201	57.834	16.806	59.588	1.00	8.36		N
ANISOU	7667	N	ASP B 201	1033	1105	1038	124	41	149	N
ATOM	7669	CA	ASP B 201	56.974	15.661	59.413	1.00	9.10		C
ANISOU	7669	CA	ASP B 201	1124	1242	1090	119	88	-29	C
ATOM	7671	CB	ASP B 201	55.925	15.556	60.522	1.00	9.39		C
ANISOU	7671	CB	ASP B 201	1066	1240	1260	-63	172	178	C
ATOM	7674	CG	ASP B 201	56.477	15.093	61.867	1.00	12.60		C
ANISOU	7674	CG	ASP B 201	1400	1909	1477	-34	-2	91	C
ATOM	7675	OD1	ASP B 201	57.668	14.661	61.985	1.00	14.53		O
ANISOU	7675	OD1	ASP B 201	1823	2155	1541	197	134	-158	O
ATOM	7676	OD2	ASP B 201	55.703	15.025	62.884	1.00	15.41		O
ANISOU	7676	OD2	ASP B 201	2349	1932	1572	365	174	10	O
ATOM	7677	C	ASP B 201	56.260	15.824	58.078	1.00	8.87		C
ANISOU	7677	C	ASP B 201	993	1218	1157	81	91	59	C
ATOM	7678	O	ASP B 201	55.957	14.832	57.401	1.00	8.40		O
ANISOU	7678	O	ASP B 201	940	1123	1126	99	267	114	O
ATOM	7679	N	VAL B 202	55.922	17.066	57.724	1.00	8.76		N
ANISOU	7679	N	VAL B 202	1072	1119	1135	34	24	15	N
ATOM	7681	CA	VAL B 202	55.333	17.301	56.397	1.00	9.57		C
ANISOU	7681	CA	VAL B 202	1250	1173	1212	23	11	43	C
ATOM	7683	CB	VAL B 202	55.047	18.801	56.148	1.00	9.03		C
ANISOU	7683	CB	VAL B 202	1197	1134	1097	12	-21	10	C
ATOM	7685	CG1	VAL B 202	54.641	19.053	54.692	1.00	9.40		C
ANISOU	7685	CG1	VAL B 202	1040	1250	1280	-102	27	36	C
ATOM	7689	CG2	VAL B 202	53.990	19.293	57.092	1.00	9.82		C
ANISOU	7689	CG2	VAL B 202	1239	1238	1250	194	-51	73	C
ATOM	7693	C	VAL B 202	56.297	16.810	55.316	1.00	9.16		C
ANISOU	7693	C	VAL B 202	1101	1159	1217	59	20	23	C
ATOM	7694	O	VAL B 202	55.938	16.072	54.366	1.00	7.77		O
ANISOU	7694	O	VAL B 202	891	894	1165	186	205	-26	O

ATOM	7695	N	ASN B 203	57.525	17.287	55.426	1.00	10.20		N
ANISOU	7695	N	ASN B 203	1302	1239	1333	64	14	-4	N
ATOM	7697	CA	ASN B 203	58.559	16.932	54.459	1.00	10.05		C
ANISOU	7697	CA	ASN B 203	1273	1280	1265	10	44	32	C
ATOM	7699	CB	ASN B 203	59.814	17.761	54.717	1.00	10.06		C
ANISOU	7699	CB	ASN B 203	1169	1280	1374	111	-23	-38	C
ATOM	7702	CG	ASN B 203	59.591	19.248	54.475	1.00	9.17		C
ANISOU	7702	CG	ASN B 203	1014	1298	1171	30	140	104	C
ATOM	7703	OD1	ASN B 203	58.694	19.637	53.713	1.00	9.46		O
ANISOU	7703	OD1	ASN B 203	1124	931	1536	66	150	653	O
ATOM	7704	ND2	ASN B 203	60.311	20.072	55.210	1.00	9.01		N
ANISOU	7704	ND2	ASN B 203	1000	1014	1408	70	245	288	N
ATOM	7707	C	ASN B 203	58.824	15.410	54.397	1.00	10.07		C
ANISOU	7707	C	ASN B 203	1267	1271	1287	66	57	33	C
ATOM	7708	O	ASN B 203	59.045	14.835	53.304	1.00	9.53		O
ANISOU	7708	O	ASN B 203	1488	915	1217	-72	-123	-25	O
ATOM	7709	N	ARG B 204	58.714	14.732	55.533	1.00	10.01		N
ANISOU	7709	N	ARG B 204	1312	1309	1180	35	-10	59	N
ATOM	7711	CA	ARG B 204	58.923	13.268	55.555	1.00	10.11		C
ANISOU	7711	CA	ARG B 204	1265	1314	1259	70	48	-37	C
ATOM	7713	CB	ARG B 204	58.977	12.709	56.936	1.00	11.25		C
ANISOU	7713	CB	ARG B 204	1473	1394	1406	98	-75	-10	C
ATOM	7716	CG	ARG B 204	59.583	11.276	56.991	1.00	14.37		C
ANISOU	7716	CG	ARG B 204	2004	1721	1736	124	-69	2	C
ATOM	7719	CD	ARG B 204	59.765	10.779	58.410	1.00	14.47		C
ANISOU	7719	CD	ARG B 204	1880	1818	1799	12	-1	45	C
ATOM	7722	NE	ARG B 204	60.674	11.630	59.176	1.00	12.17		N
ANISOU	7722	NE	ARG B 204	1179	1653	1788	-15	109	109	N
ATOM	7724	CZ	ARG B 204	60.301	12.484	60.095	1.00	11.97		C
ANISOU	7724	CZ	ARG B 204	1438	1628	1479	-95	67	86	C
ATOM	7725	NH1	ARG B 204	59.017	12.602	60.429	1.00	12.86		N
ANISOU	7725	NH1	ARG B 204	1369	1644	1870	71	58	-102	N
ATOM	7728	NH2	ARG B 204	61.193	13.185	60.741	1.00	12.50		N
ANISOU	7728	NH2	ARG B 204	1488	1615	1645	-257	213	229	N
ATOM	7731	C	ARG B 204	57.807	12.534	54.827	1.00	9.34		C
ANISOU	7731	C	ARG B 204	1158	1284	1105	58	31	51	C
ATOM	7732	O	ARG B 204	58.044	11.532	54.188	1.00	8.66		O
ANISOU	7732	O	ARG B 204	812	1232	1246	19	-159	79	O
ATOM	7733	N	ALA B 205	56.596	13.095	54.872	1.00	8.96		N
ANISOU	7733	N	ALA B 205	1110	1348	944	113	34	37	N
ATOM	7735	CA	ALA B 205	55.483	12.514	54.168	1.00	9.38		C
ANISOU	7735	CA	ALA B 205	1208	1133	1221	40	42	42	C
ATOM	7737	CB	ALA B 205	54.142	13.182	54.587	1.00	9.65		C
ANISOU	7737	CB	ALA B 205	1331	1203	1132	124	16	-13	C
ATOM	7741	C	ALA B 205	55.717	12.586	52.665	1.00	9.54		C
ANISOU	7741	C	ALA B 205	1218	1185	1222	82	-41	18	C
ATOM	7743	N	TYR B 206	56.213	13.729	52.185	1.00	8.59		N
ANISOU	7743	N	TYR B 206	1099	1071	1090	67	58	-39	N
ATOM	7745	CA	TYR B 206	56.653	13.830	50.783	1.00	8.50		C
ANISOU	7745	CA	TYR B 206	1014	1125	1088	91	-101	65	C
ATOM	7747	CB	TYR B 206	57.045	15.246	50.528	1.00	7.20		C
ANISOU	7747	CB	TYR B 206	878	926	930	192	-77	-35	C
ATOM	7750	CG	TYR B 206	55.839	16.176	50.139	1.00	7.95		C
ANISOU	7750	CG	TYR B 206	748	1088	1184	9	-74	133	C
ATOM	7751	CD1	TYR B 206	55.285	17.033	51.071	1.00	5.99		C
ANISOU	7751	CD1	TYR B 206	628	728	921	-102	-74	154	C
ATOM	7753	CE1	TYR B 206	54.216	17.899	50.746	1.00	7.13		C
ANISOU	7753	CE1	TYR B 206	996	855	858	28	69	-43	C
ATOM	7762	C	TYR B 206	57.821	12.875	50.421	1.00	8.12		C
ANISOU	7762	C	TYR B 206	1099	910	1075	-23	24	44	C
ATOM	7764	N	LEU B 207	58.781	12.777	51.307	1.00	7.46		N

ANISOU	7764	N	LEU	B	207	994	765	1072	-66	23	93	N
ATOM	7766	CA	LEU	B	207	59.949	11.942	51.047	1.00	9.84		C
ANISOU	7766	CA	LEU	B	207	1348	1125	1264	-20	-20	22	C
ATOM	7768	CB	LEU	B	207	60.944	12.060	52.198	1.00	9.38		C
ANISOU	7768	CB	LEU	B	207	1252	1127	1185	-92	6	14	C
ATOM	7771	CG	LEU	B	207	62.252	11.247	52.119	1.00	11.73		C
ANISOU	7771	CG	LEU	B	207	1481	1539	1434	23	0	65	C
ATOM	7773	CD1	LEU	B	207	63.058	11.655	50.933	1.00	12.98		C
ANISOU	7773	CD1	LEU	B	207	1434	1828	1668	119	-11	174	C
ATOM	7777	CD2	LEU	B	207	63.086	11.353	53.387	1.00	13.39		C
ANISOU	7777	CD2	LEU	B	207	1517	1725	1844	-78	-98	47	C
ATOM	7848	CA	LEU	B	212	60.552	15.519	48.012	1.00	7.58		C
ANISOU	7848	CA	LEU	B	212	951	952	975	80	57	56	C
ATOM	7850	CB	LEU	B	212	60.977	15.250	49.440	1.00	8.80		C
ANISOU	7850	CB	LEU	B	212	1126	1076	1139	127	-59	63	C
ATOM	7853	CG	LEU	B	212	61.711	16.320	50.217	1.00	8.98		C
ANISOU	7853	CG	LEU	B	212	1254	1088	1070	-1	-47	93	C
ATOM	7855	CD1	LEU	B	212	60.861	17.534	50.455	1.00	8.85		C
ANISOU	7855	CD1	LEU	B	212	954	1309	1097	-37	24	-51	C
ATOM	7859	CD2	LEU	B	212	62.288	15.776	51.576	1.00	10.09		C
ANISOU	7859	CD2	LEU	B	212	943	1628	1262	51	-25	129	C
ATOM	7863	C	LEU	B	212	61.815	15.786	47.229	1.00	7.10		C
ANISOU	7863	C	LEU	B	212	766	895	1034	18	-23	24	C
ATOM	7865	N	SER	B	213	61.913	16.976	46.696	1.00	7.08		N
ANISOU	7865	N	SER	B	213	674	925	1090	-11	-47	-55	N
ATOM	7874	C	SER	B	213	63.971	18.198	47.116	1.00	7.04		C
ANISOU	7874	C	SER	B	213	877	1011	787	23	-55	-22	C
ATOM	7875	O	SER	B	213	63.527	19.266	47.564	1.00	8.08		O
ANISOU	7875	O	SER	B	213	1033	1179	858	-38	4	-193	O
ATOM	7876	N	VAL	B	214	65.176	17.725	47.420	1.00	7.32		N
ANISOU	7876	N	VAL	B	214	907	960	914	-22	27	-86	N
ATOM	7878	CA	VAL	B	214	66.065	18.412	48.332	1.00	8.50		C
ANISOU	7878	CA	VAL	B	214	992	1117	1118	26	-31	7	C
ATOM	7880	CB	VAL	B	214	66.662	17.473	49.325	1.00	9.49		C
ANISOU	7880	CB	VAL	B	214	1135	1234	1236	-41	-99	20	C
ATOM	7882	CG1	VAL	B	214	67.640	18.265	50.220	1.00	9.17		C
ANISOU	7882	CG1	VAL	B	214	1216	1187	1081	158	-197	-2	C
ATOM	7886	CG2	VAL	B	214	65.557	16.808	50.137	1.00	11.30		C
ANISOU	7886	CG2	VAL	B	214	1389	1327	1576	58	-56	153	C
ATOM	7890	C	VAL	B	214	67.181	18.986	47.493	1.00	8.26		C
ANISOU	7890	C	VAL	B	214	916	1055	1164	-59	-44	-4	C
ATOM	7891	O	VAL	B	214	67.989	18.241	46.905	1.00	9.17		O
ANISOU	7891	O	VAL	B	214	800	1215	1469	-74	237	171	O
ATOM	7892	N	GLU	B	215	67.172	20.293	47.357	1.00	8.23		N
ANISOU	7892	N	GLU	B	215	917	1057	1150	26	-148	-24	N
ATOM	7894	CA	GLU	B	215	68.211	20.975	46.602	1.00	9.54		C
ANISOU	7894	CA	GLU	B	215	1134	1246	1244	5	1	10	C
ATOM	7896	CB	GLU	B	215	67.662	22.184	45.830	1.00	10.10		C
ANISOU	7896	CB	GLU	B	215	1238	1336	1261	-114	-15	54	C
ATOM	7905	C	GLU	B	215	69.311	21.454	47.534	1.00	10.31		C
ANISOU	7905	C	GLU	B	215	1285	1363	1268	-32	-7	35	C
ATOM	7906	O	GLU	B	215	69.015	21.990	48.613	1.00	10.95		O
ANISOU	7906	O	GLU	B	215	1164	1485	1511	-3	42	-262	O
ATOM	7907	N	ILE	B	216	70.582	21.269	47.143	1.00	8.84		N
ANISOU	7907	N	ILE	B	216	1186	1120	1050	17	136	-41	N
ATOM	7909	CA	ILE	B	216	71.663	21.828	47.943	1.00	9.55		C
ANISOU	7909	CA	ILE	B	216	1186	1120	1323	-38	53	154	C
ATOM	7911	CB	ILE	B	216	73.019	21.179	47.676	1.00	9.77		C
ANISOU	7911	CB	ILE	B	216	1333	987	1390	-102	84	95	C
ATOM	7916	CD1	ILE	B	216	72.520	19.201	49.103	1.00	12.05		C
ANISOU	7916	CD1	ILE	B	216	1598	1323	1658	92	147	24	C

ATOM	7920	CG2	ILE	B	216	74.070	21.754	48.722	1.00	13.23		C
ANISOU	7920	CG2	ILE	B	216	1725	1640	1660	77	-40	68	C
ATOM	7924	C	ILE	B	216	71.764	23.376	47.628	1.00	9.10		C
ANISOU	7924	C	ILE	B	216	1022	1150	1284	-74	58	42	C
ATOM	7926	N	MET	B	217	71.750	24.157	48.702	1.00	7.68		N
ANISOU	7926	N	MET	B	217	609	1083	1225	-68	47	-9	N
ATOM	7928	CA	MET	B	217	72.067	25.557	48.649	1.00	8.58		C
ANISOU	7928	CA	MET	B	217	947	1130	1180	11	-66	39	C
ATOM	7930	CB	MET	B	217	71.215	26.316	49.614	1.00	9.01		C
ANISOU	7930	CB	MET	B	217	1087	1149	1187	-42	-41	-31	C
ATOM	7933	CG	MET	B	217	71.532	27.850	49.786	1.00	10.49		C
ANISOU	7933	CG	MET	B	217	1444	1082	1457	-75	-43	172	C
ATOM	7936	SD	MET	B	217	70.285	28.672	50.856	1.00	12.06		S
ANISOU	7936	SD	MET	B	217	1553	1472	1554	196	-5	-92	S
ATOM	7937	CE	MET	B	217	68.809	28.514	49.872	1.00	13.78		C
ANISOU	7937	CE	MET	B	217	1799	1689	1747	-59	188	138	C
ATOM	7941	C	MET	B	217	73.554	25.671	49.012	1.00	7.98		C
ANISOU	7941	C	MET	B	217	960	984	1088	-4	-22	-25	C
ATOM	7942	O	MET	B	217	73.983	25.471	50.156	1.00	9.87		O
ANISOU	7942	O	MET	B	217	1136	1378	1233	46	-49	97	O
ATOM	7985	CB	TYR	B	221	73.672	30.854	49.426	1.00	7.23		C
ANISOU	7985	CB	TYR	B	221	960	899	887	60	-74	86	C
ATOM	8000	C	TYR	B	221	75.110	31.869	51.094	1.00	8.55		C
ANISOU	8000	C	TYR	B	221	1222	1053	971	35	-17	-38	C
ATOM	8001	O	TYR	B	221	75.737	31.045	51.754	1.00	9.15		O
ANISOU	8001	O	TYR	B	221	1659	1026	790	301	-188	-143	O
ATOM	8002	N	ALA	B	222	74.590	32.977	51.612	1.00	8.75		N
ANISOU	8002	N	ALA	B	222	1042	1052	1230	134	29	102	N
ATOM	8004	CA	ALA	B	222	74.490	33.151	53.032	1.00	9.59		C
ANISOU	8004	CA	ALA	B	222	1092	1207	1344	87	-1	51	C
ATOM	8006	CB	ALA	B	222	74.801	34.548	53.454	1.00	11.40		C
ANISOU	8006	CB	ALA	B	222	1295	1475	1559	-94	103	-38	C
ATOM	8010	C	ALA	B	222	73.055	32.801	53.417	1.00	10.24		C
ANISOU	8010	C	ALA	B	222	1158	1337	1395	-75	98	121	C
ATOM	8011	O	ALA	B	222	72.111	33.257	52.772	1.00	8.71		O
ANISOU	8011	O	ALA	B	222	748	1108	1453	-277	191	100	O
ATOM	8012	N	TRP	B	223	72.927	31.966	54.433	1.00	10.57		N
ANISOU	8012	N	TRP	B	223	1245	1424	1345	17	81	91	N
ATOM	8014	CA	TRP	B	223	71.617	31.648	55.060	1.00	9.73		C
ANISOU	8014	CA	TRP	B	223	1096	1348	1250	-25	-9	12	C
ATOM	8016	CB	TRP	B	223	71.184	30.192	54.891	1.00	10.75		C
ANISOU	8016	CB	TRP	B	223	1287	1554	1243	-72	26	34	C
ATOM	8019	CG	TRP	B	223	69.899	29.871	55.706	1.00	8.42		C
ANISOU	8019	CG	TRP	B	223	965	1209	1024	-108	-24	-124	C
ATOM	8020	CD1	TRP	B	223	68.777	30.564	55.722	1.00	11.01		C
ANISOU	8020	CD1	TRP	B	223	1576	1392	1216	-25	-62	78	C
ATOM	8022	NE1	TRP	B	223	67.868	30.014	56.604	1.00	10.77		N
ANISOU	8022	NE1	TRP	B	223	1066	1479	1544	-85	238	46	N
ATOM	8024	CE2	TRP	B	223	68.482	28.978	57.262	1.00	9.41		C
ANISOU	8024	CE2	TRP	B	223	1173	1284	1116	88	205	-33	C
ATOM	8025	CD2	TRP	B	223	69.753	28.847	56.705	1.00	10.61		C
ANISOU	8025	CD2	TRP	B	223	1055	1431	1545	-103	35	2	C
ATOM	8026	CE3	TRP	B	223	70.584	27.825	57.182	1.00	10.23		C
ANISOU	8026	CE3	TRP	B	223	1311	1107	1466	-59	-10	144	C
ATOM	8028	CZ3	TRP	B	223	70.117	26.979	58.160	1.00	9.84		C
ANISOU	8028	CZ3	TRP	B	223	1148	1407	1182	45	95	-61	C
ATOM	8030	CH2	TRP	B	223	68.855	27.118	58.669	1.00	8.97		C
ANISOU	8030	CH2	TRP	B	223	956	1151	1300	-287	314	189	C
ATOM	8032	CZ2	TRP	B	223	68.006	28.095	58.219	1.00	9.05		C
ANISOU	8032	CZ2	TRP	B	223	1018	1072	1348	-71	74	-65	C
ATOM	8034	C	TRP	B	223	71.869	31.908	56.530	1.00	12.21		C

ANISOU	8034	C	TRP	B	223	1507	1706	1426	23	106	131	C
ATOM	8035	O	TRP	B	223	72.679	31.207	57.206	1.00	12.56		O
ANISOU	8035	O	TRP	B	223	1512	1769	1490	191	130	164	O
ATOM	8036	N	LEU	B	224	71.202	32.910	57.044	1.00	13.37		N
ANISOU	8036	N	LEU	B	224	1845	1630	1605	125	-8	85	N
ATOM	8038	CA	LEU	B	224	71.365	33.268	58.431	1.00	16.15		C
ANISOU	8038	CA	LEU	B	224	2148	1939	2046	20	-24	-15	C
ATOM	8040	CB	LEU	B	224	71.968	34.652	58.499	1.00	15.97		C
ANISOU	8040	CB	LEU	B	224	2147	1959	1960	3	-41	62	C
ATOM	8043	CG	LEU	B	224	73.181	34.812	57.629	1.00	16.95		C
ANISOU	8043	CG	LEU	B	224	2208	2006	2223	-30	-11	-31	C
ATOM	8045	CD1	LEU	B	224	73.511	36.294	57.545	1.00	17.91		C
ANISOU	8045	CD1	LEU	B	224	2639	2042	2123	-104	95	-78	C
ATOM	8049	CD2	LEU	B	224	74.332	33.994	58.192	1.00	16.82		C
ANISOU	8049	CD2	LEU	B	224	2057	2028	2304	-97	-33	-44	C
ATOM	8053	C	LEU	B	224	70.001	33.280	59.080	1.00	17.40		C
ANISOU	8053	C	LEU	B	224	2296	2140	2172	-5	24	11	C
ATOM	8054	O	LEU	B	224	68.990	33.461	58.434	1.00	17.58		O
ANISOU	8054	O	LEU	B	224	2358	2193	2125	-82	128	51	O
ATOM	8055	N	ASP	B	225	69.972	33.108	60.384	1.00	20.27		N
ANISOU	8055	N	ASP	B	225	2661	2523	2518	-43	22	-61	N
ATOM	8057	CA	ASP	B	225	68.730	33.298	61.076	1.00	21.74		C
ANISOU	8057	CA	ASP	B	225	2821	2776	2662	-5	-8	-70	C
ATOM	8059	CB	ASP	B	225	68.103	31.958	61.370	1.00	24.35		C
ANISOU	8059	CB	ASP	B	225	3126	3088	3038	-132	73	-32	C
ATOM	8062	CG	ASP	B	225	68.286	31.510	62.753	1.00	27.20		C
ANISOU	8062	CG	ASP	B	225	3643	3475	3213	-41	-155	58	C
ATOM	8063	OD1	ASP	B	225	67.837	32.209	63.661	1.00	28.91		O
ANISOU	8063	OD1	ASP	B	225	4029	3334	3622	57	179	16	O
ATOM	8064	OD2	ASP	B	225	68.776	30.406	62.998	1.00	35.41		O
ANISOU	8064	OD2	ASP	B	225	4537	4026	4890	256	-187	-74	O
ATOM	8065	C	ASP	B	225	68.953	34.252	62.271	1.00	20.97		C
ANISOU	8065	C	ASP	B	225	2675	2670	2623	-20	25	-96	C
ATOM	8066	O	ASP	B	225	69.994	34.295	62.892	1.00	19.64		O
ANISOU	8066	O	ASP	B	225	2782	2562	2117	99	-4	-326	O
ATOM	8067	N	THR	B	226	67.989	35.112	62.462	1.00	21.71		N
ANISOU	8067	N	THR	B	226	2736	2756	2757	-64	-22	-61	N
ATOM	8069	CA	THR	B	226	68.089	36.091	63.502	1.00	22.49		C
ANISOU	8069	CA	THR	B	226	2811	2826	2905	-36	-3	-27	C
ATOM	8071	CB	THR	B	226	67.423	37.337	63.054	1.00	23.27		C
ANISOU	8071	CB	THR	B	226	2843	2945	3053	-12	-38	9	C
ATOM	8073	OG1	THR	B	226	65.995	37.123	63.017	1.00	25.90		O
ANISOU	8073	OG1	THR	B	226	2876	3306	3656	-164	94	193	O
ATOM	8075	CG2	THR	B	226	67.810	37.653	61.618	1.00	22.07		C
ANISOU	8075	CG2	THR	B	226	2778	2765	2841	-22	-10	-42	C
ATOM	8079	C	THR	B	226	67.500	35.666	64.814	1.00	22.74		C
ANISOU	8079	C	THR	B	226	2777	2881	2981	-44	46	5	C
ATOM	8080	O	THR	B	226	67.089	36.498	65.584	1.00	23.28		O
ANISOU	8080	O	THR	B	226	2840	2889	3116	-69	102	16	O
ATOM	8081	N	GLY	B	227	67.607	34.401	65.160	1.00	23.41		N
ANISOU	8081	N	GLY	B	227	3006	2911	2978	-153	91	-18	N
ATOM	8083	CA	GLY	B	227	67.015	33.944	66.426	1.00	23.57		C
ANISOU	8083	CA	GLY	B	227	3046	2993	2915	-78	19	-36	C
ATOM	8086	C	GLY	B	227	67.648	34.275	67.769	1.00	22.92		C
ANISOU	8086	C	GLY	B	227	3004	2895	2808	-46	133	-59	C
ATOM	8087	O	GLY	B	227	66.902	34.104	68.749	1.00	23.27		O
ANISOU	8087	O	GLY	B	227	3199	2856	2787	-100	309	-211	O
ATOM	8088	N	THR	B	228	68.974	34.570	67.831	1.00	20.30		N
ANISOU	8088	N	THR	B	228	2837	2456	2419	-190	118	-77	N
ATOM	8090	CA	THR	B	228	69.693	34.910	69.038	1.00	19.39		C
ANISOU	8090	CA	THR	B	228	2617	2246	2501	-142	75	58	C

ATOM	8092	CB	THR	B	228	70.895	34.051	69.304	1.00	19.57		C
ANISOU	8092	CB	THR	B	228	2629	2279	2527	-94	91	-61	C
ATOM	8094	OG1	THR	B	228	71.812	34.144	68.199	1.00	21.77		O
ANISOU	8094	OG1	THR	B	228	3277	2154	2841	-117	367	50	O
ATOM	8096	CG2	THR	B	228	70.526	32.524	69.512	1.00	20.69		C
ANISOU	8096	CG2	THR	B	228	2719	2534	2608	-101	76	90	C
ATOM	8100	C	THR	B	228	70.188	36.343	68.959	1.00	17.65		C
ANISOU	8100	C	THR	B	228	2403	2118	2185	-176	-1	-26	C
ATOM	8101	O	THR	B	228	70.216	36.958	67.898	1.00	15.76		O
ANISOU	8101	O	THR	B	228	2356	1620	2009	-393	-14	76	O
ATOM	8102	N	HIS	B	229	70.563	36.882	70.104	1.00	16.06		N
ANISOU	8102	N	HIS	B	229	2218	1857	2024	-167	23	8	N
ATOM	8104	CA	HIS	B	229	71.014	38.257	70.095	1.00	14.52		C
ANISOU	8104	CA	HIS	B	229	1963	1683	1870	-48	-14	-29	C
ATOM	8106	CB	HIS	B	229	71.367	38.720	71.493	1.00	12.98		C
ANISOU	8106	CB	HIS	B	229	1851	1417	1661	-165	-8	-107	C
ATOM	8109	CG	HIS	B	229	70.228	38.719	72.432	1.00	10.75		C
ANISOU	8109	CG	HIS	B	229	1570	998	1515	-106	-125	-118	C
ATOM	8110	ND1	HIS	B	229	70.306	38.140	73.687	1.00	12.38		N
ANISOU	8110	ND1	HIS	B	229	1719	1435	1551	141	121	-129	N
ATOM	8112	CE1	HIS	B	229	69.188	38.392	74.341	1.00	13.36		C
ANISOU	8112	CE1	HIS	B	229	1596	1672	1807	-1	58	52	C
ATOM	8114	NE2	HIS	B	229	68.403	39.115	73.561	1.00	11.34		N
ANISOU	8114	NE2	HIS	B	229	1629	1145	1532	-24	-25	-34	N
ATOM	8116	CD2	HIS	B	229	68.985	39.232	72.329	1.00	10.57		C
ANISOU	8116	CD2	HIS	B	229	1711	980	1322	-127	-33	-94	C
ATOM	8118	C	HIS	B	229	72.231	38.368	69.260	1.00	13.81		C
ANISOU	8118	C	HIS	B	229	1919	1611	1714	-12	66	-69	C
ATOM	8119	O	HIS	B	229	72.391	39.322	68.535	1.00	13.96		O
ANISOU	8119	O	HIS	B	229	2023	1474	1807	68	225	-164	O
ATOM	8120	N	ASP	B	230	73.129	37.408	69.420	1.00	13.86		N
ANISOU	8120	N	ASP	B	230	1791	1682	1790	-25	21	26	N
ATOM	8122	CA	ASP	B	230	74.367	37.415	68.663	1.00	15.10		C
ANISOU	8122	CA	ASP	B	230	1984	1860	1890	-21	38	28	C
ATOM	8124	CB	ASP	B	230	75.299	36.287	69.112	1.00	15.54		C
ANISOU	8124	CB	ASP	B	230	1969	1958	1978	12	44	85	C
ATOM	8130	C	ASP	B	230	74.135	37.259	67.186	1.00	14.28		C
ANISOU	8130	C	ASP	B	230	1804	1803	1818	-101	15	2	C
ATOM	8131	O	ASP	B	230	74.811	37.912	66.392	1.00	14.14		O
ANISOU	8131	O	ASP	B	230	1804	1661	1907	-126	45	122	O
ATOM	8132	N	SER	B	231	73.234	36.341	66.805	1.00	14.19		N
ANISOU	8132	N	SER	B	231	1809	1725	1855	-115	101	-1	N
ATOM	8134	CA	SER	B	231	72.978	36.049	65.396	1.00	13.24		C
ANISOU	8134	CA	SER	B	231	1611	1638	1780	-69	9	3	C
ATOM	8136	CB	SER	B	231	72.173	34.683	65.203	1.00	14.74		C
ANISOU	8136	CB	SER	B	231	1844	1772	1983	7	-42	-128	C
ATOM	8139	OG	SER	B	231	70.734	34.754	65.306	1.00	15.47		O
ANISOU	8139	OG	SER	B	231	1822	1945	2109	-76	153	-73	O
ATOM	8141	C	SER	B	231	72.380	37.308	64.708	1.00	12.47		C
ANISOU	8141	C	SER	B	231	1639	1431	1666	-63	70	-57	C
ATOM	8142	O	SER	B	231	72.682	37.597	63.536	1.00	11.46		O
ANISOU	8142	O	SER	B	231	1785	951	1618	-23	365	-156	O
ATOM	8143	N	LEU	B	232	71.473	38.004	65.392	1.00	10.76		N
ANISOU	8143	N	LEU	B	232	1542	1254	1292	-141	79	-144	N
ATOM	8145	CA	LEU	B	232	70.833	39.173	64.828	1.00	10.71		C
ANISOU	8145	CA	LEU	B	232	1301	1471	1295	-28	-12	-63	C
ATOM	8147	CB	LEU	B	232	69.674	39.600	65.742	1.00	12.65		C
ANISOU	8147	CB	LEU	B	232	1586	1662	1558	-31	41	-10	C
ATOM	8150	CG	LEU	B	232	68.974	40.917	65.467	1.00	13.28		C
ANISOU	8150	CG	LEU	B	232	1497	1844	1702	-19	55	-64	C
ATOM	8152	CD1	LEU	B	232	68.267	40.897	64.154	1.00	16.56		C

ANISOU	8152	CD1	LEU	B	232	1673	2449	2168	-162	39	38	C
ATOM	8156	CD2	LEU	B	232	68.084	41.261	66.676	1.00	12.73		C
ANISOU	8156	CD2	LEU	B	232	1179	1800	1858	-90	-37	33	C
ATOM	8160	C	LEU	B	232	71.868	40.286	64.594	1.00	11.07		C
ANISOU	8160	C	LEU	B	232	1453	1408	1344	-28	-70	-4	C
ATOM	8161	O	LEU	B	232	71.887	40.941	63.561	1.00	9.66		O
ANISOU	8161	O	LEU	B	232	1185	1208	1275	-82	-64	-59	O
ATOM	8162	N	LEU	B	233	72.812	40.429	65.515	1.00	10.93		N
ANISOU	8162	N	LEU	B	233	1423	1425	1302	-80	71	-36	N
ATOM	8196	N	ALA	B	235	73.908	39.354	61.533	1.00	9.24		N
ANISOU	8196	N	ALA	B	235	1317	1086	1107	89	112	55	N
ATOM	8198	CA	ALA	B	235	73.177	39.535	60.316	1.00	10.26		C
ANISOU	8198	CA	ALA	B	235	1340	1204	1354	-31	-10	-55	C
ATOM	8200	CB	ALA	B	235	71.761	39.087	60.487	1.00	9.61		C
ANISOU	8200	CB	ALA	B	235	1306	1066	1276	-30	64	-27	C
ATOM	17420	O	THR	D	240	79.115	33.191	59.546	1.00	9.27		O
ANISOU	17420	O	THR	D	240	1167	1036	1319	-98	-359	-259	O
ATOM	17467	C	ASN	D	243	79.478	29.829	61.792	1.00	10.18		C
ANISOU	17467	C	ASN	D	243	1366	1222	1279	48	21	71	C
ATOM	17468	O	ASN	D	243	79.019	28.935	62.519	1.00	10.23		O
ANISOU	17468	O	ASN	D	243	1155	1331	1399	225	13	377	O
ATOM	17469	N	ARG	D	244	78.789	30.286	60.760	1.00	9.26		N
ANISOU	17469	N	ARG	D	244	1248	1121	1149	17	-22	89	N
ATOM	17471	CA	ARG	D	244	77.483	29.788	60.455	1.00	9.26		C
ANISOU	17471	CA	ARG	D	244	1298	1041	1176	0	-27	34	C
ATOM	17473	CB	ARG	D	244	76.769	30.790	59.523	1.00	10.39		C
ANISOU	17473	CB	ARG	D	244	1359	1239	1349	37	-78	5	C
ATOM	17476	CG	ARG	D	244	75.417	30.298	58.996	1.00	11.21		C
ANISOU	17476	CG	ARG	D	244	1637	1282	1339	47	-103	-6	C
ATOM	17479	CD	ARG	D	244	74.430	30.138	60.075	1.00	11.36		C
ANISOU	17479	CD	ARG	D	244	1341	1381	1595	-33	51	39	C
ATOM	17482	NE	ARG	D	244	73.085	30.023	59.624	1.00	9.24		N
ANISOU	17482	NE	ARG	D	244	1461	1237	810	284	49	-161	N
ATOM	17484	CZ	ARG	D	244	72.069	29.775	60.415	1.00	11.87		C
ANISOU	17484	CZ	ARG	D	244	1364	1731	1416	-199	-60	-86	C
ATOM	17485	NH1	ARG	D	244	72.255	29.524	61.720	1.00	13.92		N
ANISOU	17485	NH1	ARG	D	244	1288	2228	1772	10	-98	315	N
ATOM	17488	NH2	ARG	D	244	70.850	29.797	59.913	1.00	9.39		N
ANISOU	17488	NH2	ARG	D	244	909	1649	1009	210	306	-109	N
ATOM	17491	C	ARG	D	244	77.586	28.425	59.761	1.00	8.39		C
ANISOU	17491	C	ARG	D	244	1119	991	1078	38	-63	16	C
ATOM	17492	O	ARG	D	244	76.885	27.462	60.115	1.00	7.53		O
ANISOU	17492	O	ARG	D	244	1172	682	1004	-41	21	-26	O
ATOM	17493	N	GLN	D	245	78.520	28.342	58.845	1.00	8.85		N
ANISOU	17493	N	GLN	D	245	1270	947	1144	-53	-41	2	N
ATOM	17495	CA	GLN	D	245	78.627	27.167	57.941	1.00	9.62		C
ANISOU	17495	CA	GLN	D	245	1224	1151	1277	-46	-69	-52	C
ATOM	17497	CB	GLN	D	245	79.170	27.564	56.609	1.00	9.49		C
ANISOU	17497	CB	GLN	D	245	1243	1131	1230	-66	-18	-79	C
ATOM	17500	CG	GLN	D	245	78.366	28.541	55.821	1.00	9.07		C
ANISOU	17500	CG	GLN	D	245	841	1168	1435	-167	26	4	C
ATOM	17508	C	GLN	D	245	79.464	25.976	58.437	1.00	10.04		C
ANISOU	17508	C	GLN	D	245	1220	1191	1401	25	-110	-43	C
ATOM	17509	O	GLN	D	245	79.221	24.855	58.044	1.00	9.65		O
ANISOU	17509	O	GLN	D	245	1060	1283	1322	-8	-336	-52	O
ATOM	36667	O41	TDG	L	500	54.446	27.838	65.670	1.00	16.05		O
ANISOU	36667	O41	TDG	L	500	1569	2473	2054	264	289	160	O
ATOM	36668	C41	TDG	L	500	55.391	28.673	65.287	1.00	16.68		C
ANISOU	36668	C41	TDG	L	500	1976	2244	2117	89	323	108	C
ATOM	36669	N31	TDG	L	500	55.024	29.804	64.759	1.00	14.38		N
ANISOU	36669	N31	TDG	L	500	1358	2321	1785	139	395	60	N

ATOM 36671	C21	TDG L 500	55.931	30.667	64.281	1.00	15.80		C
ANISOU36671	C21	TDG L 500	1929	1930	2143	-78	10	47	C
ATOM 36672	O21	TDG L 500	55.497	31.766	63.737	1.00	14.30		O
ANISOU36672	O21	TDG L 500	1546	1580	2307	-198	326	-24	O
ATOM 36673	C51	TDG L 500	56.754	28.374	65.373	1.00	18.47		C
ANISOU36673	C51	TDG L 500	2043	2422	2551	-1	85	30	C
ATOM 36674	C5A	TDG L 500	57.220	27.088	65.971	1.00	20.79		C
ANISOU36674	C5A	TDG L 500	2525	2835	2538	29	176	142	C
ATOM 36678	C61	TDG L 500	57.671	29.264	64.819	1.00	17.12		C
ANISOU36678	C61	TDG L 500	1833	2125	2546	53	20	29	C
ATOM 36680	N11	TDG L 500	57.228	30.388	64.291	1.00	16.47		N
ANISOU36680	N11	TDG L 500	1862	2126	2268	-225	-34	56	N
ATOM 36681	C1,	TDG L 500	58.148	31.325	63.664	1.00	18.34		C
ANISOU36681	C1,	TDG L 500	2114	2433	2422	53	100	132	C
ATOM 36683	C2,	TDG L 500	59.217	31.851	64.508	1.00	19.71		C
ANISOU36683	C2,	TDG L 500	2420	2409	2657	-94	256	-170	C
ATOM 36686	O4,	TDG L 500	58.876	30.519	62.754	1.00	18.66		O
ANISOU36686	O4,	TDG L 500	2173	2250	2665	-68	-44	5	O
ATOM 36687	C4,	TDG L 500	60.207	30.990	62.749	1.00	18.80		C
ANISOU36687	C4,	TDG L 500	2303	2344	2494	17	88	-43	C
ATOM 36689	C3,	TDG L 500	60.435	32.248	63.645	1.00	18.57		C
ANISOU36689	C3,	TDG L 500	2205	2303	2548	-47	168	-42	C
ATOM 36691	O3,	TDG L 500	60.258	33.249	62.659	1.00	17.42		O
ANISOU36691	O3,	TDG L 500	2073	2270	2275	-297	315	-181	O
ATOM 36693	C5,	TDG L 500	61.088	29.811	63.095	1.00	18.43		C
ANISOU36693	C5,	TDG L 500	2244	2322	2434	98	-74	-122	C
ATOM 36696	O5,	TDG L 500	60.989	29.542	64.467	1.00	22.36		O
ANISOU36696	O5,	TDG L 500	2880	2881	2733	275	191	-158	O
ATOM 36697	P	TDG L 500	62.331	29.087	65.219	1.00	26.22		P
ANISOU36697	P	TDG L 500	3505	3033	3422	588	159	-35	P
ATOM 36698	O1P	TDG L 500	61.807	28.579	66.646	1.00	27.82		O
ANISOU36698	O1P	TDG L 500	4304	3274	2990	563	-232	83	O
ATOM 36699	O2P	TDG L 500	63.615	29.855	64.751	1.00	25.15		O
ANISOU36699	O2P	TDG L 500	3365	2913	3276	294	-221	62	O
ATOM 36700	OPP	TDG L 500	62.717	27.816	64.322	1.00	27.90		O
ANISOU36700	OPP	TDG L 500	4155	3471	2971	195	-112	-294	O
ATOM 36701	P2	TDG L 500	62.591	26.341	64.812	1.00	29.58		P
ANISOU36701	P2	TDG L 500	4200	3860	3178	-7	26	-243	P
ATOM 36702	O3P	TDG L 500	61.020	26.110	64.953	1.00	29.31		O
ANISOU36702	O3P	TDG L 500	3819	4136	3180	257	225	115	O
ATOM 36703	O4P	TDG L 500	63.661	26.033	65.922	1.00	24.37		O
ANISOU36703	O4P	TDG L 500	3580	2723	2955	18	-69	-486	O
ATOM 36704	O1	TDG L 500	63.071	25.488	63.496	1.00	19.99		O
ANISOU36704	O1	TDG L 500	3073	2037	2482	-46	-23	-123	O
ATOM 36705	C1	TDG L 500	62.328	25.527	62.258	1.00	17.60		C
ANISOU36705	C1	TDG L 500	2364	1979	2342	-69	-36	-2	C
ATOM 36707	C2	TDG L 500	62.164	24.153	61.715	1.00	13.60		C
ANISOU36707	C2	TDG L 500	1720	1793	1652	56	-136	12	C
ATOM 36709	O2	TDG L 500	61.456	23.364	62.660	1.00	13.31		O
ANISOU36709	O2	TDG L 500	1841	1856	1357	238	194	-113	O
ATOM 36711	C3	TDG L 500	63.507	23.538	61.349	1.00	12.52		C
ANISOU36711	C3	TDG L 500	1659	1829	1266	26	-45	31	C
ATOM 36713	O3	TDG L 500	63.226	22.327	60.641	1.00	12.02		O
ANISOU36713	O3	TDG L 500	1688	1740	1136	-108	516	-75	O
ATOM 36715	C4	TDG L 500	64.318	24.529	60.539	1.00	13.54		C
ANISOU36715	C4	TDG L 500	1641	1694	1809	83	-23	29	C
ATOM 36717	O4	TDG L 500	65.621	24.046	60.272	1.00	10.48		O
ANISOU36717	O4	TDG L 500	1078	1363	1541	72	-249	494	O
ATOM 36719	C5	TDG L 500	64.470	25.920	61.165	1.00	16.65		C
ANISOU36719	C5	TDG L 500	2262	2094	1969	108	102	-31	C
ATOM 36721	O5	TDG L 500	63.228	26.415	61.567	1.00	17.26		O

ANISOU36721	O5	TDG	L	500	1951	2339	2266	-60	174	8	O
ATOM 36722	C6	TDG	L	500	64.967	26.933	60.143	1.00	15.14		C
ANISOU36722	C6	TDG	L	500	1943	1879	1928	96	78	-16	C
ATOM 36725	O6	TDG	L	500	65.056	28.265	60.654	1.00	16.12		O
ANISOU36725	O6	TDG	L	500	2163	1934	2024	171	-258	70	O
ATOM 37512	S	SO4	B	700	62.058	31.485	70.618	1.00	53.92		S
ANISOU37512	S	SO4	B	700	6820	6777	6889	-172	3	-96	S
ATOM 37513	O1	SO4	B	700	61.130	32.036	71.597	1.00	52.22		O
ANISOU37513	O1	SO4	B	700	6626	6481	6732	-73	-42	-42	O
ATOM 37514	O2	SO4	B	700	62.105	30.029	70.771	1.00	55.88		O
ANISOU37514	O2	SO4	B	700	7153	6931	7146	28	37	40	O
ATOM 37515	O3	SO4	B	700	61.531	31.799	69.278	1.00	54.98		O
ANISOU37515	O3	SO4	B	700	6988	6870	7029	-96	66	94	O
ATOM 37516	O4	SO4	B	700	63.438	31.980	70.796	1.00	53.10		O
ANISOU37516	O4	SO4	B	700	6659	6740	6777	4	47	-49	O
ATOM 37527	O5	CIT	E	1	69.575	33.835	75.731	1.00	36.63		O
ANISOU37527	O5	CIT	E	1	4868	4636	4412	-11	2	-49	O
ATOM 37528	C6	CIT	E	1	70.791	33.888	75.416	1.00	39.35		C
ANISOU37528	C6	CIT	E	1	4981	4998	4970	-12	18	23	C
ATOM 37529	O6	CIT	E	1	71.247	32.998	74.674	1.00	41.58		O
ANISOU37529	O6	CIT	E	1	5266	5111	5422	35	80	17	O
ATOM 37531	C3	CIT	E	1	71.718	34.993	75.900	1.00	39.47		C
ANISOU37531	C3	CIT	E	1	5003	5011	4981	-34	-14	-31	C
ATOM 37534	C4	CIT	E	1	72.232	35.805	74.701	1.00	39.05		C
ANISOU37534	C4	CIT	E	1	4897	5038	4900	18	-48	-36	C
ATOM 37614	O	HOH	I	18	75.994	24.384	51.895	1.00	11.33		O
ANISOU37614	O	HOH	I	18	1664	1593	1047	-215	167	-22	O
ATOM 37647	O	HOH	I	29	69.846	13.685	61.690	1.00	15.13		O
ANISOU37647	O	HOH	I	29	2063	1510	2174	128	377	-197	O
ATOM 37668	O	HOH	I	36	76.863	26.212	53.757	1.00	9.98		O
ANISOU37668	O	HOH	I	36	1199	1323	1268	-66	-33	170	O
ATOM 37680	O	HOH	I	40	64.904	35.880	53.349	1.00	17.08		O
ANISOU37680	O	HOH	I	40	2598	2067	1824	30	-347	-142	O
ATOM 37701	O	HOH	I	47	77.668	16.261	56.572	1.00	20.19		O
ANISOU37701	O	HOH	I	47	2668	2473	2530	119	84	212	O
ATOM 37719	O	HOH	I	53	47.557	27.708	67.146	1.00	18.50		O
ANISOU37719	O	HOH	I	53	2525	2302	2200	-154	134	-122	O
ATOM 37740	O	HOH	I	60	71.149	41.852	68.585	1.00	16.78		O
ANISOU37740	O	HOH	I	60	2932	2082	1359	-29	-19	-230	O
ATOM 37773	O	HOH	I	71	43.346	30.828	55.249	1.00	15.85		O
ANISOU37773	O	HOH	I	71	1508	2701	1812	82	305	-91	O
ATOM 37788	O	HOH	I	76	62.294	19.912	57.381	1.00	12.75		O
ANISOU37788	O	HOH	I	76	1448	1729	1668	-99	-37	182	O
ATOM 37803	O	HOH	I	81	68.499	13.187	59.247	1.00	13.36		O
ANISOU37803	O	HOH	I	81	1789	1385	1901	206	125	212	O
ATOM 37818	O	HOH	I	86	63.131	10.442	57.959	1.00	16.21		O
ANISOU37818	O	HOH	I	86	1655	1692	2812	-149	125	110	O
ATOM 37953	O	HOH	I	131	66.650	37.845	52.521	1.00	16.65		O
ANISOU37953	O	HOH	I	131	2378	2237	1711	285	-40	-100	O
ATOM 38043	O	HOH	I	161	70.030	10.989	65.274	1.00	24.84		O
ANISOU38043	O	HOH	I	161	3597	2513	3327	7	-365	150	O
ATOM 38052	O	HOH	I	164	63.244	22.509	57.989	1.00	11.26		O
ANISOU38052	O	HOH	I	164	1245	1879	1151	265	104	4	O
ATOM 38064	O	HOH	I	168	64.424	24.683	52.860	1.00	13.22		O
ANISOU38064	O	HOH	I	168	1669	2056	1298	113	54	-362	O
ATOM 38118	O	HOH	I	186	73.717	35.735	61.533	1.00	19.65		O
ANISOU38118	O	HOH	I	186	2692	2625	2147	-294	252	-240	O
ATOM 38148	O	HOH	I	196	53.881	16.917	63.619	1.00	16.26		O
ANISOU38148	O	HOH	I	196	1583	2145	2448	-536	140	-32	O
ATOM 38154	O	HOH	I	198	65.463	37.846	49.824	1.00	22.03		O
ANISOU38154	O	HOH	I	198	2698	2814	2858	87	-60	796	O

ATOM 38163	O	HOH I 201	47.058	18.330	62.254	1.00	26.88		O
ANISOU38163	O	HOH I 201	3265	3527	3418	42	445	-11	O
ATOM 38334	O	HOH I 258	69.808	35.222	72.438	1.00	24.62		O
ANISOU38334	O	HOH I 258	3745	2789	2818	-409	102	51	O
ATOM 38346	O	HOH I 262	50.813	21.155	68.244	1.00	26.04		O
ANISOU38346	O	HOH I 262	3008	3367	3517	194	513	281	O
ATOM 38361	O	HOH I 267	62.711	47.610	62.362	1.00	24.59		O
ANISOU38361	O	HOH I 267	3274	2644	3422	70	-234	58	O
ATOM 38445	O	HOH I 295	53.113	32.228	66.808	1.00	20.26		O
ANISOU38445	O	HOH I 295	2166	2797	2733	-288	308	-232	O
ATOM 38499	O	HOH I 313	59.399	21.295	62.197	1.00	25.28		O
ANISOU38499	O	HOH I 313	2737	4099	2766	-583	-165	224	O
ATOM 38589	O	HOH I 343	51.022	32.526	68.454	1.00	21.81		O
ANISOU38589	O	HOH I 343	2945	2819	2521	-69	357	-9	O
ATOM 38598	O	HOH I 346	72.696	33.012	61.616	1.00	19.19		O
ANISOU38598	O	HOH I 346	2474	2770	2047	-342	-553	-264	O
ATOM 38664	O	HOH I 368	57.245	23.427	64.260	1.00	18.33		O
ANISOU38664	O	HOH I 368	1806	2443	2715	127	280	389	O
ATOM 38766	O	HOH I 402	75.227	26.990	62.330	1.00	23.67		O
ANISOU38766	O	HOH I 402	2836	3702	2453	-132	-306	-308	O
ATOM 38793	O	HOH I 411	43.770	31.241	63.622	1.00	27.56		O
ANISOU38793	O	HOH I 411	3588	3638	3244	-132	186	-444	O
ATOM 38796	O	HOH I 412	67.213	13.851	69.612	1.00	24.16		O
ANISOU38796	O	HOH I 412	2850	3149	3180	-252	87	347	O
ATOM 38802	O	HOH I 414	78.149	33.255	62.147	1.00	20.45		O
ANISOU38802	O	HOH I 414	2877	2503	2390	-204	336	229	O
ATOM 38823	O	HOH I 421	49.500	38.544	60.745	1.00	21.54		O
ANISOU38823	O	HOH I 421	2870	3024	2288	232	445	155	O
ATOM 38826	O	HOH I 422	46.316	19.931	64.291	1.00	31.72		O
ANISOU38826	O	HOH I 422	4227	4019	3804	-132	425	-152	O
ATOM 38952	O	HOH I 464	59.068	37.526	68.769	1.00	26.15		O
ANISOU38952	O	HOH I 464	3620	3246	3071	-420	179	348	O
ATOM 39012	O	HOH I 484	73.214	35.582	71.694	1.00	28.62		O
ANISOU39012	O	HOH I 484	4127	3198	3548	60	410	199	O
ATOM 39042	O	HOH I 494	61.261	33.077	80.107	1.00	27.22		O
ANISOU39042	O	HOH I 494	3618	3389	3333	81	-128	61	O
ATOM 39069	O	HOH I 503	76.871	28.406	63.906	1.00	30.69		O
ANISOU39069	O	HOH I 503	4007	3976	3677	-1	227	160	O
ATOM 39186	O	HOH I 542	54.835	12.482	58.354	1.00	23.19		O
ANISOU39186	O	HOH I 542	3262	2611	2937	-213	572	128	O
ATOM 39192	O	HOH I 544	66.833	35.998	76.703	1.00	36.39		O
ANISOU39192	O	HOH I 544	4425	4633	4768	10	37	207	O
ATOM 39348	O	HOH I 596	51.741	33.727	71.143	1.00	31.08		O
ANISOU39348	O	HOH I 596	4166	3803	3838	148	-256	5	O
ATOM 39501	O	HOH I 647	43.892	28.398	64.444	1.00	25.32		O
ANISOU39501	O	HOH I 647	3314	3122	3185	-77	177	-107	O
ATOM 39528	O	HOH I 656	59.610	15.996	62.937	1.00	25.80		O
ANISOU39528	O	HOH I 656	2606	3359	3837	-13	388	183	O
ATOM 39579	O	HOH I 673	60.352	22.045	66.279	1.00	22.69		O
ANISOU39579	O	HOH I 673	2775	2480	3365	-108	-39	54	O
ATOM 39627	O	HOH I 689	75.989	34.827	62.792	1.00	38.42		O
ANISOU39627	O	HOH I 689	5023	4713	4858	299	6	-9	O
ATOM 39666	O	HOH I 702	46.506	18.258	66.442	1.00	39.21		O
ANISOU39666	O	HOH I 702	4778	5310	4809	-43	113	146	O
ATOM 39747	O	HOH I 729	69.594	12.210	67.695	1.00	21.58		O
ANISOU39747	O	HOH I 729	3088	2410	2702	-251	74	354	O
ATOM 39783	O	HOH I 741	42.253	24.456	58.180	1.00	25.06		O
ANISOU39783	O	HOH I 741	2738	3467	3313	33	89	186	O
ATOM 39819	O	HOH I 753	66.393	26.476	65.077	1.00	25.41		O
ANISOU39819	O	HOH I 753	3501	3100	3053	334	-432	144	O
ATOM 39843	O	HOH I 761	55.756	37.559	66.590	1.00	30.32		O

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ANISOU39843	O	HOH I 761	4217	3354	3949	168	384	-52	O
ATOM 40152	O	HOH I 864	64.716	14.353	66.359	1.00	27.30		O
ANISOU40152	O	HOH I 864	3341	3496	3534	-187	-159	341	O
ATOM 40182	O	HOH I 874	41.524	29.286	67.937	1.00	34.86		O
ANISOU40182	O	HOH I 874	3934	4683	4628	-179	295	-47	O
ATOM 40191	O	HOH I 877	60.831	22.658	68.376	1.00	34.79		O
ANISOU40191	O	HOH I 877	4213	4634	4369	75	35	214	O
ATOM 40248	O	HOH I 896	64.308	19.693	70.526	1.00	35.61		O
ANISOU40248	O	HOH I 896	4582	4508	4439	-33	74	-140	O
ATOM 40344	O	HOH I 928	47.296	24.563	68.734	1.00	31.14		O
ANISOU40344	O	HOH I 928	3868	4559	3403	114	257	55	O
ATOM 40356	O	HOH I 932	79.944	21.840	60.235	1.00	29.91		O
ANISOU40356	O	HOH I 932	3908	3445	4011	86	18	114	O
ATOM 40359	O	HOH I 933	74.063	26.028	64.165	1.00	29.56		O
ANISOU40359	O	HOH I 933	3599	3330	4302	-216	-219	-30	O
ATOM 40440	O	HOH I 960	67.907	44.590	65.913	1.00	25.75		O
ANISOU40440	O	HOH I 960	3991	3123	2667	307	-94	-102	O
ATOM 40524	O	HOH I 988	44.680	28.076	71.141	1.00	32.07		O
ANISOU40524	O	HOH I 988	3615	4563	4007	90	246	71	O
ATOM 40527	O	HOH I 989	76.881	18.522	65.404	1.00	36.15		O
ANISOU40527	O	HOH I 989	4732	4581	4420	18	-47	203	O
ATOM 40545	O	HOH I 995	71.412	31.739	64.211	1.00	37.83		O
ANISOU40545	O	HOH I 995	5510	4309	4554	-88	-88	-98	O
ATOM 40650	O	HOH I1030	43.085	35.179	61.829	1.00	29.31		O
ANISOU40650	O	HOH I1030	3512	4074	3550	-146	328	-25	O
ATOM 40680	O	HOH I1040	78.792	19.679	63.253	1.00	30.49		O
ANISOU40680	O	HOH I1040	3304	4489	3791	421	-273	-40	O
ATOM 40743	O	HOH I1061	62.083	8.368	56.141	1.00	30.31		O
ANISOU40743	O	HOH I1061	3980	3671	3864	-297	90	139	O
ATOM 41025	O	HOH I1155	45.685	27.086	64.968	1.00	34.35		O
ANISOU41025	O	HOH I1155	4377	4478	4196	172	-50	-110	O
ATOM 41028	O	HOH I1156	65.844	31.135	64.957	1.00	29.31		O
ANISOU41028	O	HOH I1156	3568	4292	3277	-1	526	71	O
ATOM 41046	O	HOH I1162	54.204	33.208	71.481	1.00	37.05		O
ANISOU41046	O	HOH I1162	4197	4861	5018	71	32	-174	O
ATOM 41070	O	HOH I1170	56.730	27.088	69.870	1.00	26.26		O
ANISOU41070	O	HOH I1170	3062	3611	3301	106	-323	-47	O
ATOM 41088	O	HOH I1176	66.289	12.662	67.402	1.00	34.69		O
ANISOU41088	O	HOH I1176	4168	4266	4745	-147	-209	277	O
ATOM 41241	O	HOH I1227	42.355	30.902	59.139	1.00	34.91		O
ANISOU41241	O	HOH I1227	4405	4832	4027	175	327	-244	O
ATOM 41277	O	HOH I1239	45.815	26.865	68.979	1.00	34.82		O
ANISOU41277	O	HOH I1239	4752	4483	3995	170	214	-26	O
ATOM 41301	O	HOH I1247	64.283	33.912	68.802	1.00	33.61		O
ANISOU41301	O	HOH I1247	4050	4800	3919	-32	124	1	O
ATOM 41328	O	HOH I1256	74.746	30.073	63.643	1.00	31.66		O
ANISOU41328	O	HOH I1256	4113	4664	3250	10	118	93	O
ATOM 41361	O	HOH I1267	46.154	22.723	64.620	1.00	32.16		O
ANISOU41361	O	HOH I1267	4122	4078	4017	-24	138	-1	O
ATOM 41844	O	HOH I1428	56.153	44.452	67.899	1.00	68.92		O
ANISOU41844	O	HOH I1428	8731	8715	8739	43	74	-5	O
ATOM 41931	O	HOH I1457	42.278	20.775	60.981	1.00	52.15		O
ANISOU41931	O	HOH I1457	6470	6727	6616	-18	125	-25	O
ATOM 42024	O	HOH I1488	43.667	25.895	66.993	1.00	49.68		O
ANISOU42024	O	HOH I1488	6441	6401	6034	29	98	15	O
ATOM 42072	O	HOH I1504	51.430	29.321	74.525	1.00	43.73		O
ANISOU42072	O	HOH I1504	5704	5261	5648	116	40	-118	O
ATOM 42189	O	HOH I1543	63.585	12.662	68.678	1.00	45.50		O
ANISOU42189	O	HOH I1543	5793	5842	5650	-96	36	39	O
ATOM 42198	O	HOH I1546	46.149	22.235	68.256	1.00	42.88		O
ANISOU42198	O	HOH I1546	5244	5352	5696	154	61	74	O

ATOM 42354	O	HOH I1598	41.897	22.955	60.273	1.00	37.01		O
ANISOU42354	O	HOH I1598	4736	4726	4600	-122	168	-74	O
ATOM 42495	O	HOH I1645	57.936	38.357	70.848	1.00	42.71		O
ANISOU42495	O	HOH I1645	5509	5307	5410	-98	-73	79	O
ATOM 42714	O	HOH I1718	45.890	25.122	63.196	1.00	29.45		O
ANISOU42714	O	HOH I1718	3607	4165	3416	-120	-55	133	O
ATOM 42903	O	HOH I1781	73.809	23.417	69.809	1.00	42.82		O
ANISOU42903	O	HOH I1781	5310	5243	5718	-10	11	-49	O
ATOM 42957	O	HOH I1799	63.112	9.029	60.250	1.00	32.25		O
ANISOU42957	O	HOH I1799	4254	4184	3813	-21	-45	149	O
ATOM 42993	O	HOH I1811	46.174	32.591	72.126	1.00	32.39		O
ANISOU42993	O	HOH I1811	3727	4381	4198	306	54	-215	O
ATOM 43110	O	HOH I1850	59.127	23.677	71.492	1.00	55.65		O
ANISOU43110	O	HOH I1850	7002	6928	7212	21	-54	-64	O
ATOM 43113	O	HOH I1851	50.062	32.026	72.770	1.00	34.54		O
ANISOU43113	O	HOH I1851	4386	4918	3817	187	109	-417	O
ATOM 43176	O	HOH I1872	55.497	43.865	71.656	1.00	49.64		O
ANISOU43176	O	HOH I1872	6514	6169	6175	-22	-13	72	O
ATOM 43227	O	HOH I1889	57.912	37.664	73.936	1.00	40.70		O
ANISOU43227	O	HOH I1889	5242	4982	5239	139	-1	229	O
ATOM 43308	O	HOH I1916	43.859	38.862	61.127	1.00	43.03		O
ANISOU43308	O	HOH I1916	5517	5336	5493	20	26	146	O
ATOM 43551	O	HOH I1997	54.920	12.722	69.483	1.00	50.81		O
ANISOU43551	O	HOH I1997	6663	6316	6326	19	-63	90	O
ATOM 43638	O	HOH I2026	59.575	34.722	67.479	1.00	42.46		O
ANISOU43638	O	HOH I2026	5354	5706	5074	-135	-43	-74	O
ATOM 43677	O	HOH I2039	60.421	28.844	72.145	1.00	46.75		O
ANISOU43677	O	HOH I2039	5824	5960	5975	-81	23	66	O
ATOM 43713	O	HOH I2051	66.641	9.265	60.413	1.00	38.20		O
ANISOU43713	O	HOH I2051	5022	4626	4866	93	40	-255	O
ATOM 43803	O	HOH I2081	68.762	18.925	69.486	1.00	33.71		O
ANISOU43803	O	HOH I2081	4047	4947	3811	127	-107	-57	O
ATOM 43824	O	HOH I2088	50.007	20.442	62.421	1.00	39.29		O
ANISOU43824	O	HOH I2088	5208	4899	4820	-187	276	96	O
ATOM 43872	O	HOH I2104	43.901	18.608	62.146	1.00	30.97		O
ANISOU43872	O	HOH I2104	3623	4213	3929	-106	378	-62	O
ATOM 43896	O	HOH I2112	59.270	31.554	78.642	1.00	45.34		O
ANISOU43896	O	HOH I2112	5475	6003	5749	27	-97	-112	O
ATOM 43899	O	HOH I2113	75.848	33.861	66.101	1.00	39.65		O
ANISOU43899	O	HOH I2113	4880	5004	5179	-85	-88	-152	O
ATOM 43902	O	HOH I2114	44.759	22.939	71.345	1.00	50.34		O
ANISOU43902	O	HOH I2114	6343	6307	6478	-67	9	95	O
ATOM 43962	O	HOH I2134	54.344	35.938	72.158	1.00	51.31		O
ANISOU43962	O	HOH I2134	6457	6482	6556	33	-16	13	O
ATOM 44097	O	HOH I2179	71.025	19.374	71.132	1.00	28.30		O
ANISOU44097	O	HOH I2179	3671	4038	3042	21	-26	-98	O
ATOM 44223	O	HOH I2221	65.453	37.557	58.489	1.00	43.47		O
ANISOU44223	O	HOH I2221	5582	5436	5498	-196	-181	40	O
ATOM 44226	O	HOH I2222	73.226	32.771	73.023	1.00	64.60		O
ANISOU44226	O	HOH I2222	8146	8188	8209	75	20	-52	O
ATOM 44265	O	HOH I2235	59.055	12.618	63.231	1.00	52.50		O
ANISOU44265	O	HOH I2235	6807	6614	6527	-99	-75	-77	O
ATOM 44280	O	HOH I2240	59.423	25.674	68.487	1.00	42.74		O
ANISOU44280	O	HOH I2240	5486	5223	5530	15	-156	23	O
ATOM 44394	O	HOH I2278	66.931	20.767	70.911	1.00	37.52		O
ANISOU44394	O	HOH I2278	4654	5168	4433	-325	232	121	O
ATOM 44547	O	HOH I2329	56.302	11.513	62.665	1.00	34.16		O
ANISOU44547	O	HOH I2329	4405	4218	4355	45	89	-33	O
ATOM 44589	O	HOH I2343	67.682	41.065	69.985	1.00	52.46		O
ANISOU44589	O	HOH I2343	6488	6755	6687	39	71	78	O
ATOM 44688	O	HOH I2376	42.482	36.027	58.782	1.00	33.76		O

ANISOU44688	O	HOH I2376	3344	4897	4584	-343	-25	131	O
ATOM 45057	O	HOH I2499	62.441	25.697	68.988	1.00	43.45		O
ANISOU45057	O	HOH I2499	5410	5569	5527	18	73	-47	O
ATOM 45210	O	HOH I2550	64.664	24.898	70.613	1.00	63.32		O
ANISOU45210	O	HOH I2550	8101	7967	7989	0	-17	35	O
ATOM 45216	O	HOH I2552	61.609	27.647	69.632	1.00	52.86		O
ANISOU45216	O	HOH I2552	6647	6624	6813	-95	-59	12	O
ATOM 45222	O	HOH I2554	51.446	12.951	63.313	1.00	32.89		O
ANISOU45222	O	HOH I2554	4197	4003	4294	-174	26	163	O
ATOM 45255	O	HOH I2565	73.299	17.756	70.832	1.00	46.42		O
ANISOU45255	O	HOH I2565	6056	5769	5810	41	-105	-68	O
ATOM 45450	O	HOH I2630	67.830	23.507	69.574	1.00	47.33		O
ANISOU45450	O	HOH I2630	5827	6179	5977	-97	93	10	O
ATOM 45507	O	HOH I2649	56.545	41.609	72.147	1.00	45.80		O
ANISOU45507	O	HOH I2649	5565	5761	6076	122	69	-71	O
ATOM 45528	O	HOH I2656	68.079	24.630	73.000	1.00	43.47		O
ANISOU45528	O	HOH I2656	5390	5451	5676	-7	-101	-16	O
ATOM 45546	O	HOH I2662	53.203	15.494	71.706	1.00	47.73		O
ANISOU45546	O	HOH I2662	5931	6247	5956	-97	127	17	O
ATOM 45552	O	HOH I2664	72.139	26.355	70.120	1.00	66.65		O
ANISOU45552	O	HOH I2664	8433	8375	8515	-35	19	20	O
ATOM 45585	O	HOH I2675	49.569	28.163	74.878	1.00	49.85		O
ANISOU45585	O	HOH I2675	6262	6313	6365	64	-43	-38	O
ATOM 45603	O	HOH I2681	56.406	11.065	60.146	1.00	33.83		O
ANISOU45603	O	HOH I2681	4194	4022	4638	-69	63	-24	O
ATOM 45633	O	HOH I2691	51.596	30.097	77.007	1.00	60.68		O
ANISOU45633	O	HOH I2691	7748	7631	7674	-37	0	3	O
ATOM 45717	O	HOH I2719	72.738	28.983	68.543	1.00	63.69		O
ANISOU45717	O	HOH I2719	8078	8045	8075	-1	-16	11	O
ATOM 45933	O	HOH I2791	72.650	24.936	61.880	1.00	45.51		O
ANISOU45933	O	HOH I2791	5697	5825	5768	59	-36	-33	O
ATOM 45996	O	HOH I2812	52.245	43.052	72.881	1.00	45.38		O
ANISOU45996	O	HOH I2812	5728	5866	5645	1	-15	-10	O
ATOM 46086	O	HOH I2842	70.833	22.382	70.704	1.00	46.92		O
ANISOU46086	O	HOH I2842	6084	6103	5640	111	22	-116	O
ATOM 46140	O	HOH I2860	76.101	31.721	63.074	1.00	51.42		O
ANISOU46140	O	HOH I2860	6715	6574	6246	-49	37	-20	O
ATOM 46203	O	HOH I2881	60.875	9.923	69.241	1.00	39.15		O
ANISOU46203	O	HOH I2881	4976	4735	5161	163	3	42	O
ATOM 46215	O	HOH I2885	62.072	14.845	70.562	1.00	48.90		O
ANISOU46215	O	HOH I2885	6005	6257	6315	-52	40	56	O
ATOM 46224	O	HOH I2888	67.153	17.681	74.494	1.00	53.05		O
ANISOU46224	O	HOH I2888	6670	6759	6726	-88	3	9	O
ATOM 46242	O	HOH I2894	50.382	35.259	75.028	1.00	46.75		O
ANISOU46242	O	HOH I2894	5778	6146	5837	90	43	115	O
ATOM 46251	O	HOH I2897	74.189	32.497	68.445	1.00	50.96		O
ANISOU46251	O	HOH I2897	6676	6134	6552	-61	-48	30	O
ATOM 46266	O	HOH I2902	51.944	36.711	76.282	1.00	61.13		O
ANISOU46266	O	HOH I2902	7753	7682	7792	2	43	9	O
ATOM 46275	O	HOH I2905	68.307	19.936	76.278	1.00	48.19		O
ANISOU46275	O	HOH I2905	5964	6205	6139	82	-21	-70	O
ATOM 46341	O	HOH I2927	61.473	15.804	72.791	1.00	67.70		O
ANISOU46341	O	HOH I2927	8549	8524	8646	17	-44	-11	O
ATOM 46347	O	HOH I2929	70.087	28.966	70.429	1.00	51.54		O
ANISOU46347	O	HOH I2929	6629	6422	6531	-79	33	31	O
ATOM 46452	O	HOH I2964	59.644	24.439	65.361	1.00	24.35		O
ANISOU46452	O	HOH I2964	2799	2670	3782	119	-492	114	O
ATOM 46455	O	HOH I2965	65.407	28.461	63.629	1.00	35.39		O
ANISOU46455	O	HOH I2965	4437	4538	4469	266	-368	-260	O
ATOM 46470	O	HOH I2970	63.893	29.687	62.345	1.00	34.97		O
ANISOU46470	O	HOH I2970	4714	4317	4255	52	139	190	O

ATOM	46509	O	HOH	I2983	57.732	30.602	70.029	1.00	52.81		O
ANISOU	46509	O	HOH	I2983	6628	6700	6735	-67	-44	22	O
ATOM	46512	O	HOH	I2984	63.472	29.428	73.612	1.00	43.98		O
ANISOU	46512	O	HOH	I2984	5677	5542	5491	-46	-1	88	O
END											

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1 Claims

2

3 1. A method of selecting agents which inhibit the
4 enzyme glucose-1-phosphate
5 thymidyltransferase (RmlA), said method
6 comprising the steps of:

7

8 a) providing a model of the active or
9 regulatory site(s) of RmlA;

10

11 b) reviewing the structure of a potential
12 inhibitory agent for at least one of these
13 sites; and

14

15 c) analysing the potential interaction of said
16 agent in said site(s).

17

18 2. A method as claimed in Claim 1 further
19 including the step of selecting an agent which
20 interacts with the active or regulatory site(s)
21 of RmlA.

22

23 3. The method as claimed in Claim 2 wherein said
24 agent binds to the active or regulatory site(s)
25 of RmlA sufficiently tightly to impede the
26 biosynthesis of rhamnose.

27

28 4. The method as claimed in either one of Claims 2
29 and 3 wherein said agent has a negative charge
30 which interacts with Arg 15 and/or Lys 25 of
31 RmlA.

32

- 1 5. The method as claimed in either one of Claims 2
2 and 3 wherein said agent has a thymidyl-like
3 moiety able to interact with Gly 10, Gln 82
4 and/or Gly 87 of RmlA.
5
- 6 6. The method as claimed in Claim 5 wherein said
7 thymidyl-like moiety forms a hydrogen bond with
8 Gly 10, Gln 82 and/or Gly 87 of RmlA.
9
- 10 7. The method as claimed in either one of Claims 2
11 and 3 wherein said agent has a glucose-like
12 moiety able to interact with Asn 111, Gly 146,
13 Glu 161, Val 172 and/or Thr 176 of RmlA.
14
- 15 8. The method as claimed in Claim 7 wherein said
16 glucose-like moiety forms a hydrogen bond with
17 Asn 111, Gly 146, Glu 161, Val 172 and/or Thr
18 176 of RmlA.
19
- 20 9. The method as claimed in any one of Claims 1 to
21 8 wherein said model of RmlA is in the form of
22 a computer data file.
23
- 24 10. The method as claimed in any one of Claims 1 to
25 9 wherein said model is based upon the X-ray
26 crystal co-ordinates of RmlA.
27
- 28 11. The method as claimed in Claim 10 wherein said
29 model includes the data for the regulatory
30 site(s) as set out in Annex 1.
31

- 1 12. The method as claimed in Claim 10 wherein said
2 model includes the data for the active site(s)
3 as set out in Annex 2.
4
- 5 13. The method as claimed in any one of Claims 1 to
6 12 wherein step b) includes providing a model
7 of the potential inhibitory agent.
8
- 9 14. The method as claimed in Claim 13 wherein said
10 model is in the form of a computer data file.
11
- 12 15. The method as claimed in any one of Claims 1 to
13 14 wherein the intermolecular interaction
14 between said agent and the model of the active
15 or regulatory site(s) of RmlA is analysed with
16 the aid of a computer.
17
- 18 16. A purified and crystallised form of the enzyme
19 glucose-1-phosphate thymidylyltransferase
20 (RmlA) obtained from *Pseudomonas aeruginosa*.
21
- 22 17. Use of the purified and crystallised form of
23 RmlA as claimed in Claim 16 to select for
24 inhibitors of said enzyme.
25
- 26 18. Use as claimed in Claim 17 wherein said
27 inhibitors inhibit the growth of *Pseudomonas*
28 *aeruginosa*.

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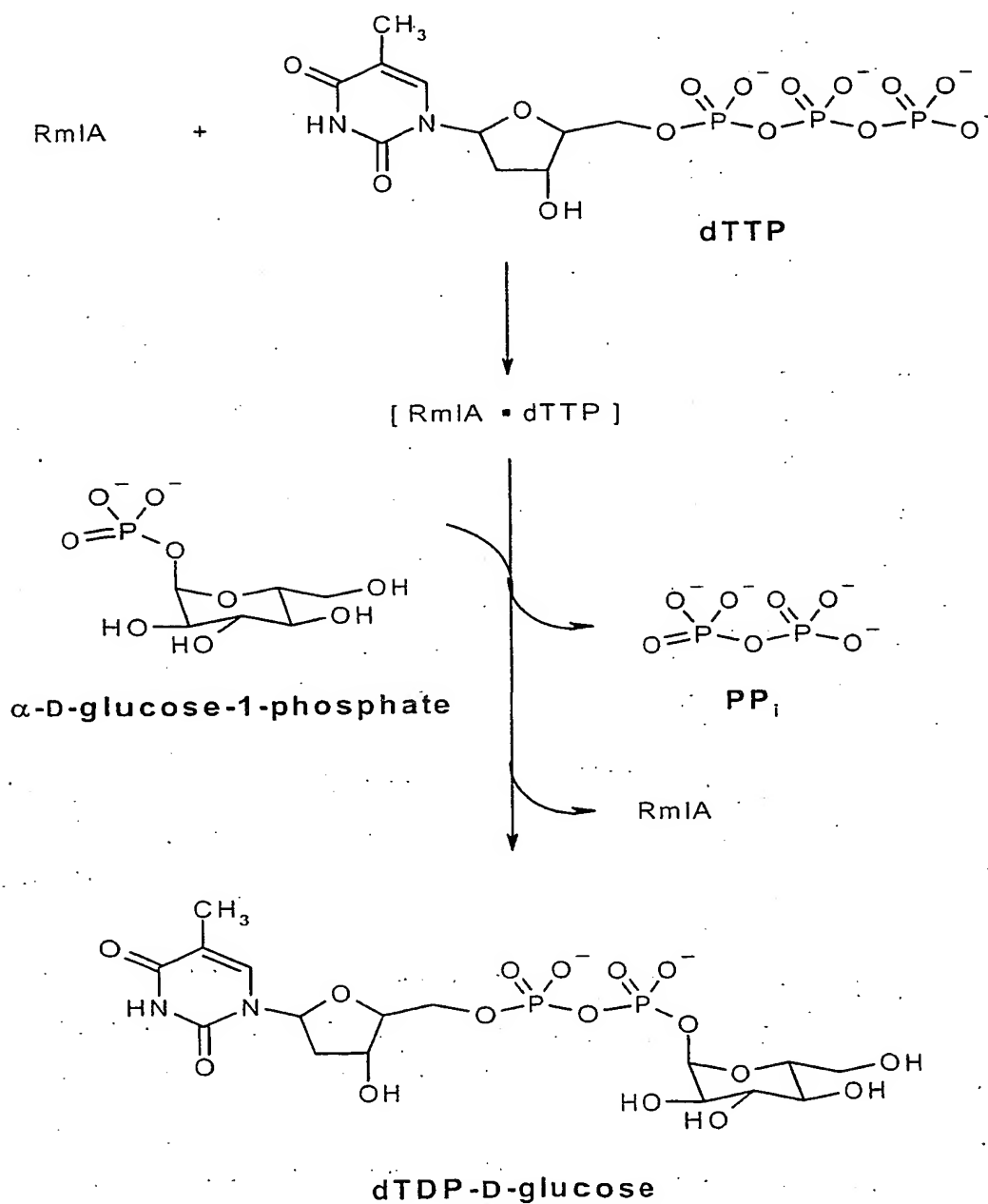


Figure 1

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Figure 2

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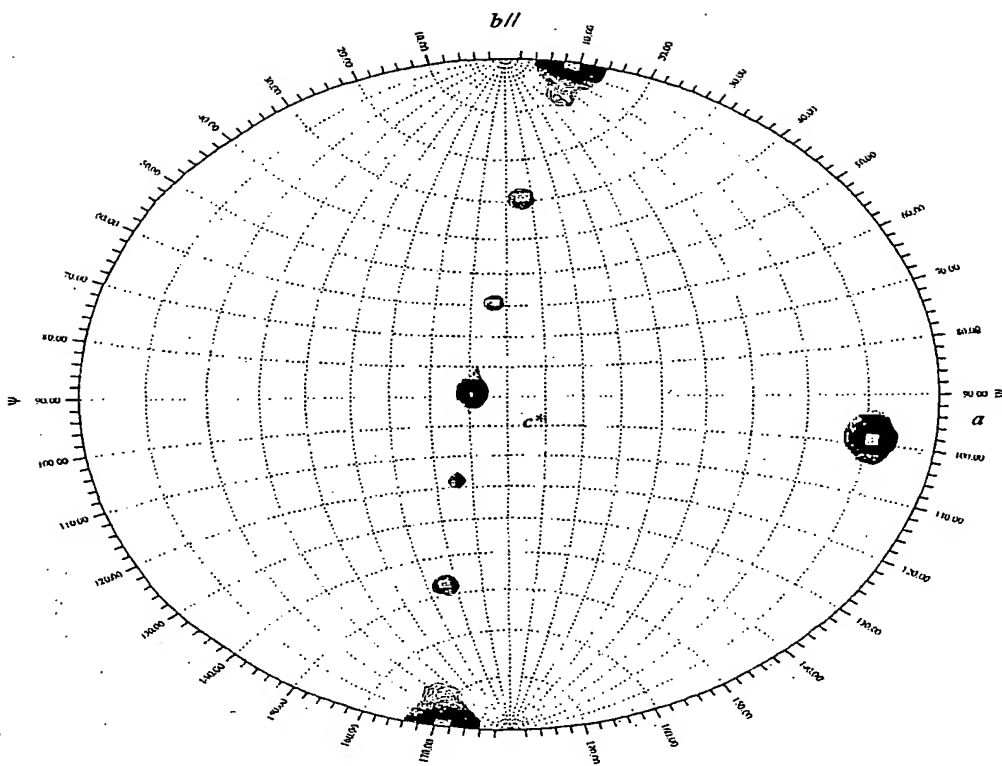


Figure 3

Table 1. Data collection statistics for non-Se-labelled RmlA crystals

Values in parentheses refer to the highest shell.					
Crystal grown in the presence of	Glucose-1-phosphate (G1P)	Glucose-1-phosphate	dTDP-glucose	G1P/thymidine/AlF ₃	dTMP
X-Ray source	rotating anode	ID14EH1	ID14EH1	ID14EH1	BM14
Wavelength (Å)	1.542	0.934	0.934	0.934	0.978
Resolution (Å)	36.27 – 2.27 (2.40 – 2.27)	40.49 – 1.90 (1.99 – 1.90)	40.49 – 1.77 (1.86 – 1.77)	36.27 – 1.87 (1.97 – 1.87)	32.12 – 1.66 (1.74 – 1.66)
Unit cell (Å; °)	a=71.6, b=73.5, c=134.2; α=89.9, β=80.8, δ=80.8	a=71.7, b=73.7, c=134.5; α=90.0, β=80.9, δ=80.9	a=71.6, b=73.4, c=134.3; α=89.9, β=80.6, δ=80.9	a=71.3, b=73.1, c=133.7; α=90.0, β=81.4, δ=81.6	a=71.5, b=73.1, c=134.7; α=89.9, β=80.9, δ=81.1
V _m (Å ³ /Da)	2.55	2.56	2.54	2.52	2.54
Total measurements	305802	377690	483036	333697	1141819
Unique reflections	116157	202988	242450	183207	297160
I/σ	6.8 (4.8)	9.2 (1.9)	7.1 (2.4)	6.9 (2.4)	10.9 (2.0)
Average redundancy	2.6 (2.3)	1.9 (1.9)	2.0 (1.3)	1.8 (1.3)	3.8 (2.0)
Completeness (%)	94.2 (84.2)	96.1 (95.6)	93.9 (77.4)	84.7 (66.8)	94.2 (81.2)
R _{merge} (%) †	6.5 (15.2)	5.4 (28.6)	7.2 (30.2)	6.7 (29.1)	5.3 (33.2)

† $R_{\text{merge}} = \sum \sum I(h)_j - \langle I(h) \rangle / \sum \sum I(h)_j$, where $I(h)$ is the measured diffraction intensity and the summation includes all observations.

Figure 4

Table 2. Data collection statistics for MAD experiment on BM14 (ESRF-Grenoble)

Values in parentheses refer to the highest shell.			
Position	Peak	Inflection	Remote
Wavelength (Å)	0.9790	0.9791	0.8855
Resolution (Å)	30.0 – 2.8 (2.87 – 2.80)		
Unit cell (Å, °)	a=71.6, b=73.9, c=133.8; α=89.8, β=80.3, δ=80.2		
V _m (Å ³ /Da)	2.54		
Total measurements	221219	220585	224654
Unique reflections	121843	121982	121112
I/σ	31.7 (9.0)	31.6 (8.8)	29.7 (9.8)
Average redundancy	1.8 (1.0)	1.8 (1.0)	1.9 (1.7)
Completeness (%)	93.0 (63.2)	93.0 (63.2)	92.7 (69.4)
R _{merge} (%) †	2.2 (8.9)	2.3 (9.5)	2.4 (8.9)

† $R_{\text{merge}} = \frac{\sum \sum I(h)_j - \langle I(h) \rangle}{\sum \sum I(h)_j}$ where $I(h)$ is the measured diffraction intensity and the summation includes all observations.

Figure 5

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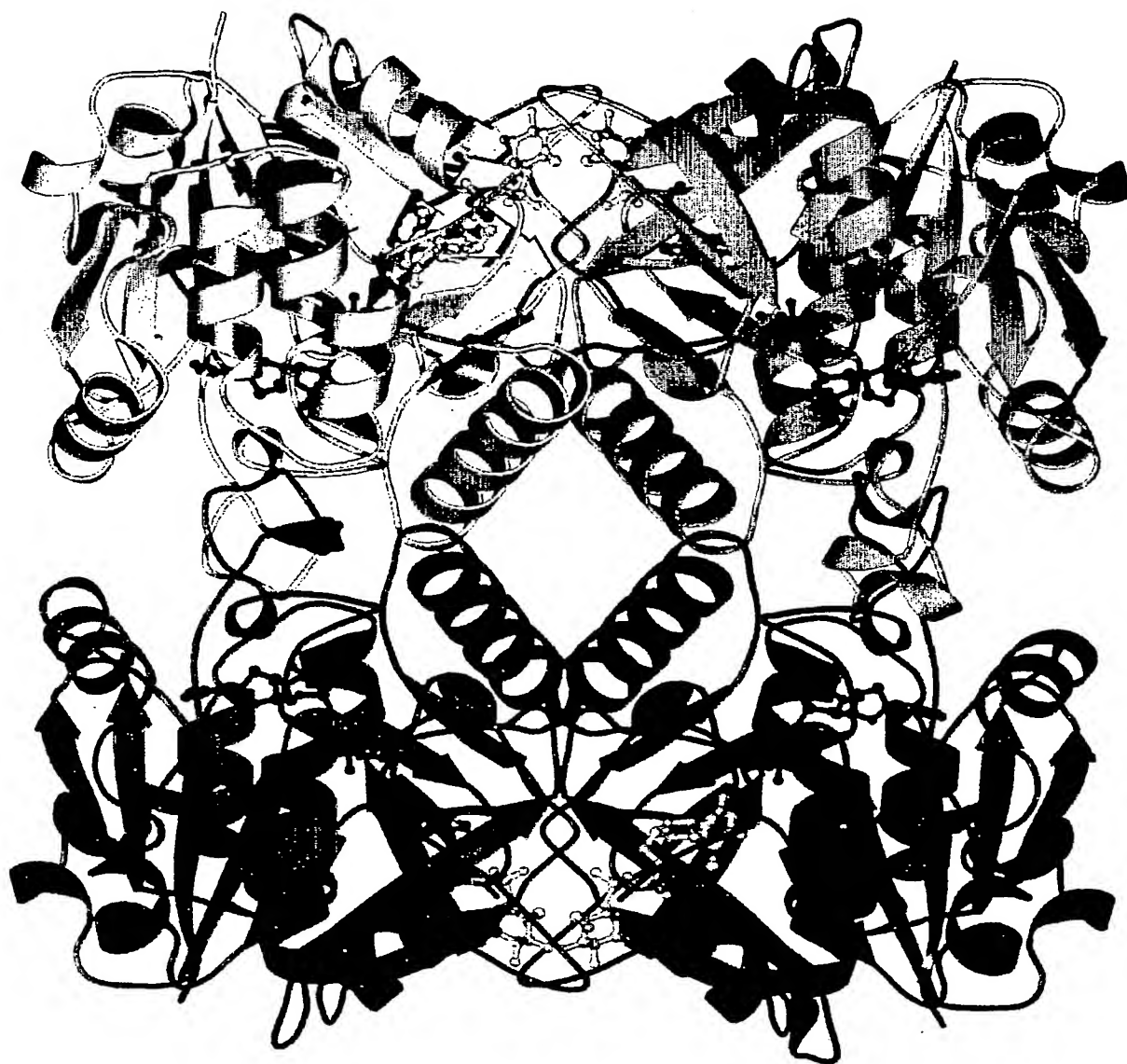


Fig. 6

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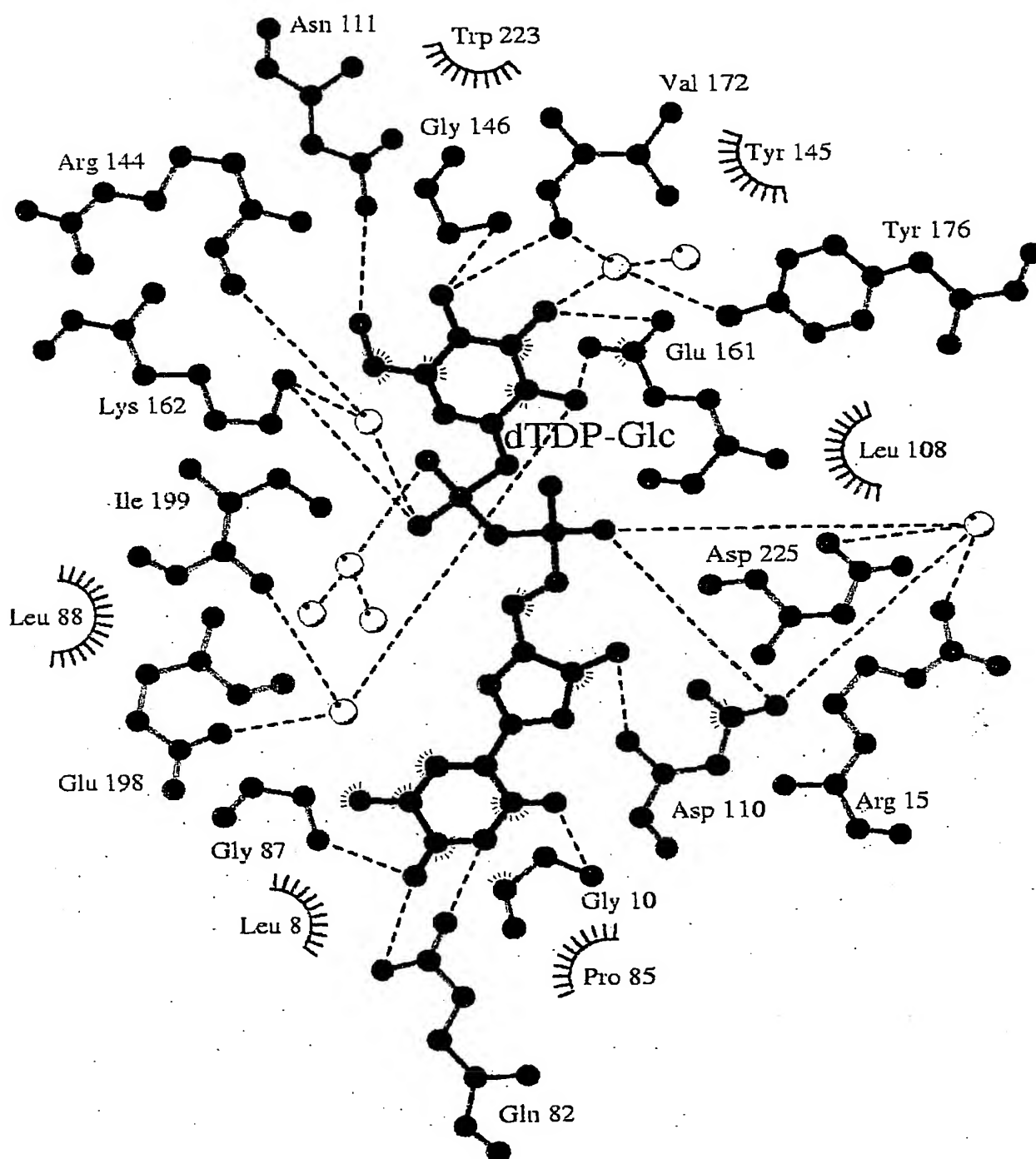
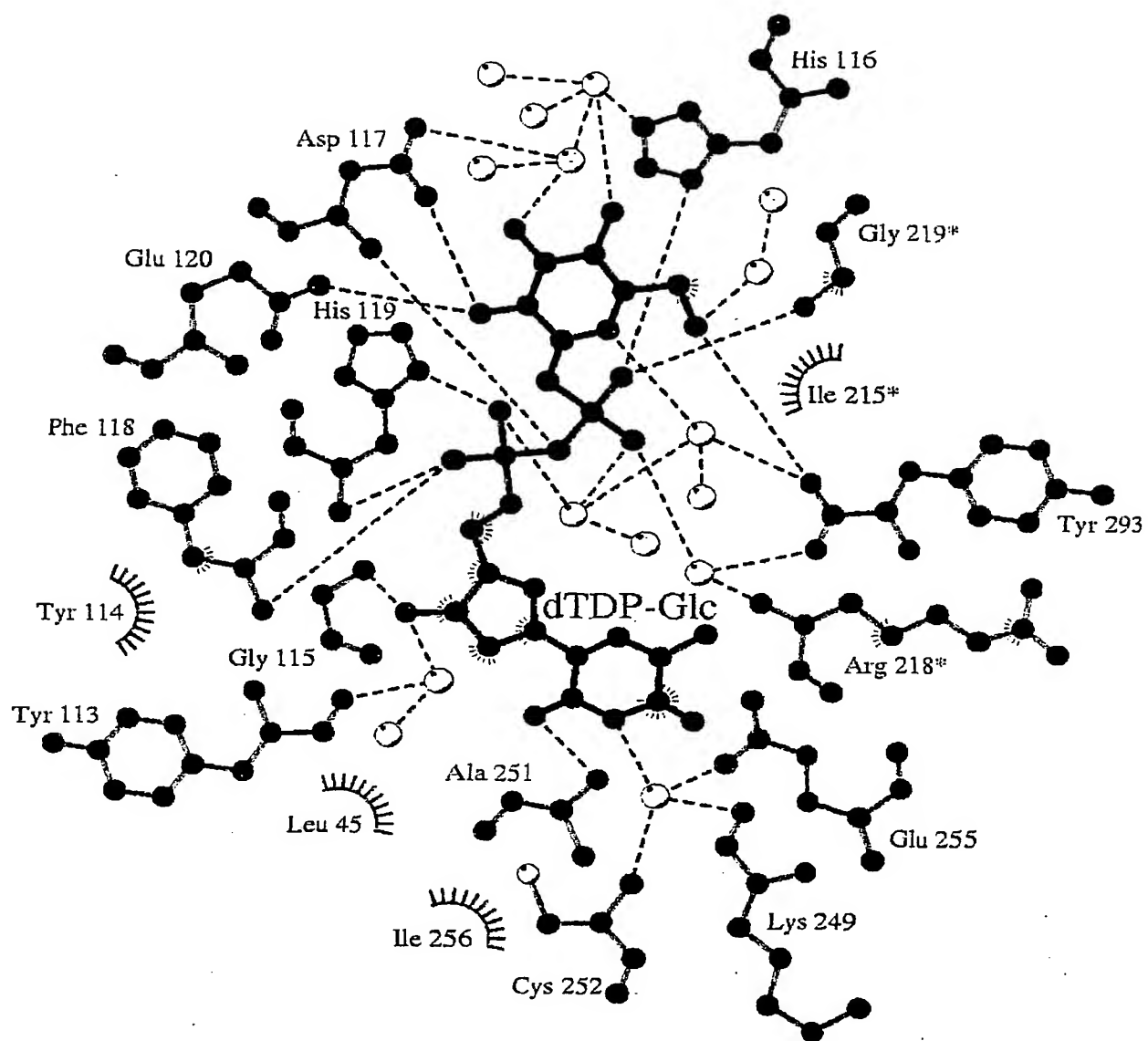


Fig. 7

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*Fig. 8*

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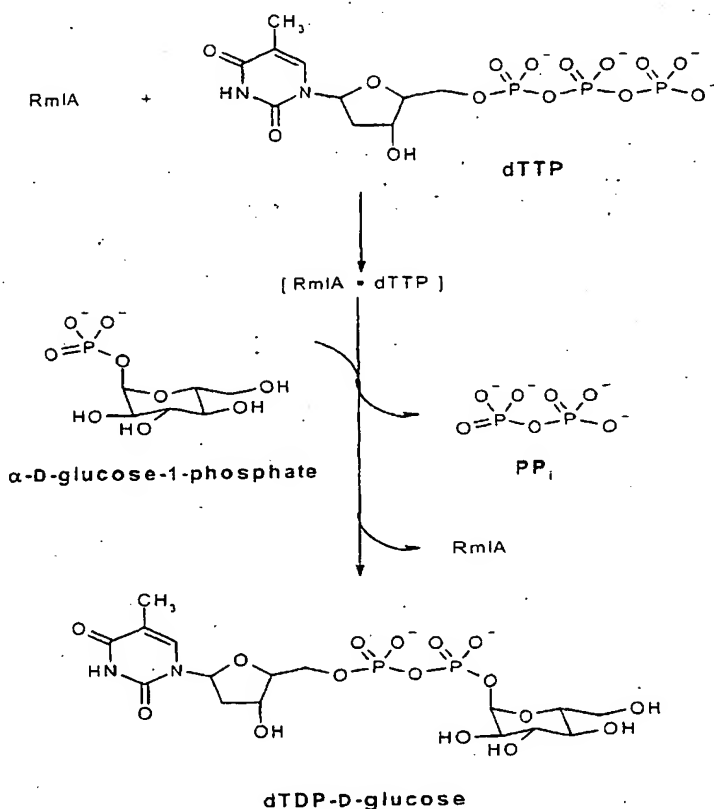
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(54) Title: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE AND METHOD FOR SELECTING INHIBITORS THEREOF



(57) Abstract: There is provided a method of obtaining selecting agents which inhibit the enzyme glucose-1-phosphate thymidyltransferase (RmlA) based upon analysis of a model of the active and regulatory site (s) of RmlA and interaction therewith by a potential inhibitory agent. The invention is based upon the provision of information on the structure of RmlA obtained through X-ray diffraction studies since a crystallised form of RmlA was obtained for the first time. The purified and crystallised form of RmlA, obtained from *Pseudomonas aeruginosa* is also described.

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Minimum documentation searched (classification system followed by classification symbols)
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Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

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CHEM ABS Data, MEDLINE, BIOSIS, EPO-Internal, WPI Data, PAJ

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	MA, YUFANG ET AL: "Determination of the pathway for rhamnose biosynthesis in mycobacteria: cloning, sequencing and expression of the Mycobacterium tuberculosis gene encoding alpha.-D-glucose-1- phosphate thymidyltransferase" MICROBIOLOGY (READING, U. K.) (1997), 143(3), 937-945 , XP008003838 the whole document --- -/--	1,16



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Patent family members are listed in annex.

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P, X	BLANKENFELDT W ET AL: "The structural basis of the catalytic mechanism and regulation of glucose-1-phosphate thymidyltransferase (RmlA)" THE EMBO JOURNAL , vol. 19, no. 24, 2000, pages 6652-6663, XP001074715 abstract -----	1-18
P, X	BLANKENFELDT, WULF ET AL: "The purification, crystallization and preliminary structural characterization of glucose-1-phosphate thymidyltransferase (RmlA), the first enzyme of the dTDP-L-rhamnose synthesis pathway from Pseudomonas aeruginosa" ACTA CRYSTALLOGRAPHICA, SECTION D: BIOLOGICAL CRYSTALLOGRAPHY (2000), D56(11), 1501-1504 , XP008003837 abstract -----	1, 16